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COMPARISON OF FINITE DIFFERENCE EXPRESSIONS
USED IN LAGRANGIAN FLUID FLOW CALCULATIONS

by

W. Herrmann
M. I. T.

TECHNICAL REPORT NO. WL-TR-64-104

Research and Technology Division
AIR FORCE WEAPONS LABORATORY
Air Force Systems Command
Kirtland Air Force Base
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FOREWORD

This technical report has been reviewed and is approved.

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ABSTRACT

A number of commonly used finite-difference analogs to partial derivatives
in two space dimensions are investigated, and a few variations are proposed.
The accuracy of these analogs is assessed by obtaining numerical results for
deformations for which the analytical gradients can be evaluated. None of
the analogs appeared superior for those deformations which were investigated,
and it appears that a choice may be made on the basis of computational con-
venience.

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v

LIST OF FIGURES

LIST OF SYMBOLS

a	Acceleration	(Eq. 2.4)*
b,c,d	Coefficients	(Eq. 2.8)
k	Constant	(Eq. 2.9)
m	Mass	(Eq. 3.3)
p	Pressure	(Eq. 2.4)
t	Time	(Eq. 2.3)
v	Volume	(Eq. 2.3)
x,z	Coordinates	(Eq. 2.1)
A	Area	(Eq. 3.2)
B,C,D,E	Functions	(Eq. 2.15)
J	Jacobian	(Eq. 2.2)
V	Volume	(Eq. 2.3)
X,Z	Coordinates	(Eq. 2.1)
γ	Symmetry Coefficient	(Eq. 3.3)
δ	Constant	(Eq. 2.9)
ρ	Density	(Eq. 2.3)

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* Numbers refer to the equation in or following which the
symbol is first introduced.

SECTION I

INTRODUCTION

One of the principal difficulties in constructing finite difference analogs to the Lagrangian equations of compressible fluid motion in two space dimensions is the choice of finite difference representation of the spatial derivatives in the momentum equation. A number of different expressions have appeared in the literature, but there seems to be little information available regarding their relative merits.

Finite difference representations of spatial gradients should introduce minimal truncation errors. However, some other properties are often considered to be more important. As a Lagrangian mesh becomes severely distorted, it is found that some finite difference expressions lead to accelerations in the wrong direction. This leads to an instability and eventual stoppage of the computer. Such severe distortions sometimes occur in relatively unimportant areas of the flow, and it is often considered more important that a finite difference expression lead to accelerations of the correct sign than of the correct absolute magnitude.

It has occasionally been argued that finite difference expressions which show large truncation errors lead to smoother solutions, and are preferable on this account. It may be noted that truncation errors serve to increase the acceleration in areas of high gradient. In this respect truncation operates in precisely the same way as artificial viscosity, which is formulated to provide an additional acceleration in areas of high gradient. It seems preferable, however, to choose the finite difference

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expression which has least truncation error, leaving smoothing of the solution to artificial viscosity terms over which one can exercise some control.

Several common finite difference expressions are discussed. In order to investigate truncation errors the following procedure was followed. A quadratic deformation was postulated, for which the density change could be found analytically using the principle of conservation of mass. On assuming an equation of state, the associated pressure change could be found analytically, and the acceleration found by applying the principle of conservation of momentum. A Murnaghan equation of state was used. The corresponding deformation of an initially square mesh was calculated for the same quadratic deformation, so that the acceleration could be computed using the finite difference expressions. The behavior of the finite difference expressions after crossing of cell vertices and after cell inversion was also investigated.

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SECTION II

DIFFERENTIAL EQUATIONS

2.1 Tensor Equations

Denote the spatial (Eulerian) coordinate x^i and the material (Lagrangian) coordinate X^I, where we use majuscules to refer to the original state, minuscules to refer to the current deformed state. At time $t=0$ take $x^i = X^I = \delta^i_I$. Consider the deformation

$$x^i = x^i \left(X^1, X^2, X^3 \right) \qquad 2.1$$

with Jacobian J given by

$$J = \left| x^i_{,I} \right| \qquad 2.2$$

where $(\quad)_{,I}$ is the covariant derivative with respect to the X^I.

The tensor equation of mass conservation is simply

$$\frac{\rho_0}{\rho} = J = \frac{dv}{dV} \qquad 2.3$$

where ρ is the density, ρ_0 the initial density at time $t=0$ and dv and dV corresponding volume elements in the deformed and undeformed states. The tensor equation of momentum conservation in a perfect fluid is

$$a_i = -\frac{1}{\rho} P_{,i} \qquad 2.4$$

where a^i is the acceleration vector, p the pressure and $(\quad)_{,i}$ is the covariant derivative with respect to the x^i. It will be useful to write this equation in the equivalent form

$$a_i = -\frac{1}{\rho} P_{,I} \, X^I_{,i} \qquad 2.5$$

or since

$$X^I_{,i} = \frac{\text{cofactor} \left(x^i_{,I} \right)}{J} \qquad 2.6$$

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$$a_i = -\frac{1}{\rho_o} p_{,I} \; cofactor(x^i_{;I}) \qquad 2.7$$

where we have used equation 2.3.

We will choose a quadratic deformation (equation 2.1) in the form

$$x^i = c^i_{JK} X^J X^K + d^i_J X^J + b^i \qquad 2.8$$

where the coefficients c^i_{JK}, d^i_J and b^i are arbitrarily chosen constants. It can be seen that the b^i introduce a uniform translation while the d^i_J introduce a homogeneous deformation and rotation. These terms do not lead to accelerations and are retained for convenience in controlling the size and position of the deformed meshes. Since we have not restricted ourselves to small deformations the c^i_{JK} and d^i_J cannot be interpreted easily as rotations and deformations, but it may be noted qualitatively that the diagonal terms introduce stretches in the corresponding coordinate directions, while the symmetric parts of the off-diagonal terms introduce shears, the anti-symmetric parts rotations. The formulation of the deformation in equation 2.8 is therefore quite flexible in producing almost any desired deformed mesh shape by appropriate choice of constants.

Once the deformation (equation 2.8) has been specified, the density distribution may be found from equation 2.3. It is necessary to postulate a relation between p and ρ before finding the acceleration. The particular form of this relation does not affect the conclusions materially. An "equation of state" in the Murnaghan form has been chosen for its simplicity

$$p = k \left\{ \left(\frac{\rho}{\rho_o} \right)^\gamma - 1 \right\}$$

or using equation 2.3

$$p = k \left(J^{-\gamma} - 1 \right) \qquad 2.9$$

4

where k and γ are material constants. We are principally concerned with relatively incompressible materials, and constants appropriate for aluminum have been used in the calculations described later (i.e. $k = 1.9 \times 10^{11} \, \mathrm{dyn/cm^2}$, $\gamma = 4$, $\rho_o = 2.78 \, \mathrm{gm/cm^3}$).

2.2 Physical Equations

Only two-dimensional rectangular Cartesian coordinates (x, z) and two-dimensional axially symmetric coordinates (x, z where we have written x for the radius) are considered. The continuity equation (equation 2.3) is usually taken in its second form

$$\frac{\rho}{\rho_o} = \frac{dv}{dV} \qquad\qquad 2.10$$

while the momentum equation (equation 2.4) takes the form

$$a_x = -\frac{1}{\rho}\frac{\partial P}{\partial x}$$

$$a_z = -\frac{1}{\rho}\frac{\partial P}{\partial z} \qquad\qquad 2.11$$

Defining $\alpha = 1$ for the rectangular case, and $\alpha = 2$ for the cylindrical case, the Jacobian for both cases may be written

$$J = \begin{vmatrix} \dfrac{\partial x}{\partial X} & 0 & \dfrac{\partial x}{\partial Z} \\[2mm] \cdot & \left(\dfrac{x}{X}\right)^{\alpha-1} & \cdot \\[2mm] \dfrac{\partial z}{\partial X} & 0 & \dfrac{\partial z}{\partial Z} \end{vmatrix} \qquad\qquad 2.12$$

Thus the alternate form of the momentum equation (equation 2.7) becomes

$$a_x = -\frac{1}{\rho_o} \left\{ \frac{\partial P}{\partial X} \frac{\partial z}{\partial Z} - \frac{\partial P}{\partial Z} \frac{\partial z}{\partial X} \right\} \left(\frac{x}{X}\right)^{\alpha-1}$$

2.13

$$a_z = -\frac{1}{\rho_o} \left\{ \frac{\partial P}{\partial Z} \frac{\partial x}{\partial X} - \frac{\partial P}{\partial X} \frac{\partial x}{\partial Z} \right\} \left(\frac{x}{X}\right)^{\alpha-1}$$

2.3 Analytical Gradients

Specializing to two-dimensional rectangular Cartesion and cylindrical polar coordinates, the deformation transformation (equation 2.8) retains only the following terms

$$x = c_{11} X^2 + c_{12} XZ + c_{13} Z^2$$

$$+ d_{11} X + d_{13} Z + b_1$$

2.14

$$z = c_{31} X^2 + c_{32} XZ + c_{33} Z^2$$

$$+ d_{31} X + d_{33} Z + b_3$$

Thus the Jacobian of the transformation can be written (from equation 2.12)

$$J = (AD - BC) E^{\alpha-1}$$

2.15

where

$$A = \frac{\partial x}{\partial X} = 2 c_{11} X + c_{12} Z + d_{11}$$

$$B = \frac{\partial x}{\partial Z} = 2 c_{13} Z + c_{12} X + d_{13}$$

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$$C = \frac{\partial z}{\partial X} = 2 c_{31} X + c_{32} Z + d_{31}$$

$$D = \frac{\partial z}{\partial Z} = 2 c_{33} Z + c_{32} X + d_{33}$$

$$E = c_{11} X + c_{12} Z + d_{11} + (c_{13} Z^2 + d_{13} Z + b_1)/X$$

Then density and pressure are given by equations 2.3 and 2.9 respectively. In order to find the accelerations, it is necessary to use the second form of the momentum equations, which may be written

$$a_x = - \frac{E^{\alpha-1}}{\rho_0} \left\{ \frac{\partial P}{\partial X} D - \frac{\partial P}{\partial Z} C \right\}$$

$$a_z = - \frac{E^{\alpha-1}}{\rho_0} \left\{ \frac{\partial P}{\partial Z} A - \frac{\partial P}{\partial X} B \right\}$$

2.16

Note that differentiation of equation 2.9 leads to

$$\frac{\partial P}{\partial X} = - \gamma k J^{-(\gamma+1)} \frac{\partial J}{\partial X}$$

$$\frac{\partial P}{\partial Z} = - \gamma k J^{-(\gamma+1)} \frac{\partial J}{\partial Z}$$

2.17

so that equations 2.16 can be conveniently written

$$a_x = \frac{\gamma k E^{\alpha-1}}{\rho_0 J^{\gamma+1}} \left\{ \frac{\partial J}{\partial X} D - \frac{\partial J}{\partial Z} C \right\}$$

2.18

$$a_z = \frac{\gamma k E^{\alpha-1}}{\rho_0 J^{\gamma+1}} \left\{ \frac{\partial J}{\partial Z} A - \frac{\partial J}{\partial X} B \right\}$$

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where the derivatives of J are easily found by differentiating equation 2.15.

Once the values of the 12 coefficients are specified in the deformation transformation (equation 2.14) it is a straightforward task to evaluate the density, pressure and accelerations at any particular point specified by its initial coordinates (X, Z).

Finally the magnitude of the acceleration vector is

$$a = \sqrt{a_r^2 + a_z^2}$$ \hfill 2.19

and the angle between the acceleration vector and the z axis is

$$\theta = \arctan \frac{a_r}{a_z}$$ \hfill 2.20

SECTION III

FINITE DIFFERENCE EXPRESSIONS

A number of finite-difference analogs to the equation of mass and momentum conservation have been evolved. An attempt is made to collect brief derivations of some of these here.

Quantities are considered only at a finite number of locations in space, initially distances ΔX and ΔZ apart. The initial X coordinate after the Ith increment ΔX is denoted X_I, and the initial Z coordinate after the Jth increment ΔZ is denoted Z_J. In effect the material is covered by a finite coordinate grid which deforms with the material (Fig. 1). Coordinates x and z at time t for the point X_I, Z_J are denoted $x_{I,J}$, $z_{I,J}$.

While positions, velocities and accelerations are considered only at the vertices of the finite difference grid, densities and pressures are considered averaged over the meshes, and are denoted $\rho_{I+\frac{1}{2}, J+\frac{1}{2}}$, etc.

In developing the finite difference equation, it is considerably more convenient to use the notation of Figure 1, translating the equation into indicial notation before programming for the computer.

3.1 Mass Equation

The second form of the mass equation

$$\rho = \rho_o \frac{dV}{dv} \qquad 3.1$$

can be set into finite difference form by considering the deformed mesh to consist of quadrilaterals. The current area of mesh 1 (Figure 1) is then

$$A_1 = \frac{1}{2} \left\{ (x_H - x_o)(z_D - z_A) - (z_H - z_o)(x_D - x_A) \right\} \qquad 3.2$$

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while the original area A_1^o at time t=0 is found by substituting X and Z for x and z in equation 3.2.

Both the rectangular Cartesian and cylindrical polar cases may be written down simultaneously by defining $\alpha = 1$ for the rectangular, $\alpha = 2$ for the cylindrical cases as before. The mass equation becomes

$$\rho_1 = \frac{m_1}{A_1 \, (\bar{x}_1)^{\alpha-1}} \qquad 3.3$$

where $\bar{x}_1$ is the radius of the centroid of the area A_1, and m_1 is a mesh constant defined as

$$m_1 = \rho_o \, A_1^o \, (\bar{X}_1)^{\alpha-1} \qquad 3.4$$

The radius of the centroid appears only in the cylindrical case. A reasonable approximation for moderate distortions is

$$\bar{x}_1 = \tfrac{1}{4} \left(x_A + x_H + x_D + x_O \right) \qquad 3.5$$
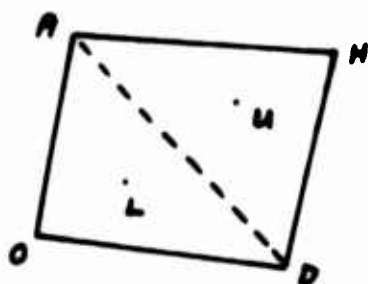
A better, but lengthier, expression may be obtained by dividing the quadrilateral into two triangles, i.e.,by taking

$$\rho_1 = \frac{m_1}{A_L \, (\bar{x}_L)^{\alpha-1} + A_u \, (\bar{x}_u)^{\alpha-1}} \qquad 3.6$$

where

$$A_u = \tfrac{1}{2} \left\{ \left(z_A - z_H \right)\!\left(x_D - x_H \right) - \left(x_A - x_H \right)\!\left(z_D - z_H \right) \right\}$$

$$A_L = \tfrac{1}{2} \left\{ \left(z_D - z_O \right)\!\left(x_A - x_O \right) - \left(x_D - x_O \right)\!\left(z_A - z_O \right) \right\}$$

$$\bar{x}_u = \tfrac{1}{3} \left(x_A + x_H + x_D \right)$$

$$\bar{x}_L = \tfrac{1}{3} \left(x_D + x_O + x_A \right)$$

and where m_1 is given by

$$m_1 = \rho_o \left\{ A_L^o \left(\bar{x}_L^o \right)^{\alpha-1} + A_u^o \left(\bar{x}_u^o \right)^{\alpha-1} \right\} \qquad 3.7$$

For the rectangular case, $\alpha = 1$, and these equations are identical to the previous ones, (equations 3.3 and 3.4).

It may be noted parenthetically, that the same results are achieved by starting with the alternate form of the mass equation (equation 2.3) as may be expected. Terms in the Jacobian (equation 2.12) may be written in finite difference form as

$$\frac{\partial x}{\partial X} = \frac{1}{\Delta X} \left(\frac{x_A + x_H}{2} - \frac{x_o + x_D}{2} \right)$$

$$\frac{\partial x}{\partial Z} = \frac{1}{\Delta Z} \left(\frac{x_H + x_D}{2} - \frac{x_A - x_o}{2} \right) \qquad 3.8$$

etc.

When these are substituted into equation 2.12, and terms are expanded and simplified, we obtain

$$J = \frac{\left(\bar{x}_1 / \bar{x}_1 \right)^{\alpha-1}}{\Delta X \Delta Z} \left\{ \left(x_H - x_o \right)\left(z_D - z_A \right) - \left(z_H - z_o \right)\left(x_D - x_A \right) \right\} \qquad 3.9$$

When this is inserted into equation 2.3, we immediately arrive again at equations 3.3 and 3.4.

3.2 Momentum Equation

A variety of difference analogs have been given for the pressure gradient terms in the momentum equations (equations 2.11). Some of these are described in the following.

3.2.1 Taylor's Expansion
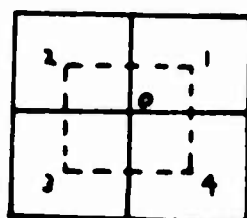
The pressure is known at discrete points 1, 2, 3, 4 surrounding point 0 at which the pressure gradients are to be evaluated.

One method is to apply Taylor's expansion between points 0 and 1, 0 and 2, etc. to obtain four equations of the form.

$$P_1 = P_0 + (x_1 - x_0) \frac{\partial P}{\partial x} + (z_1 - z_0) \frac{\partial P}{\partial z}$$

$$+ \frac{1}{2}(x_1 - x_0)^2 \frac{\partial^2 P}{\partial x^2} + \frac{1}{2}(x_1 - x_0)(z_1 - z_0) \frac{\partial^2 P}{\partial x \partial z} + \frac{1}{2}(z_1 - z_0)^2 \frac{\partial^2 P}{\partial z^2} + \cdots$$

3.10

where terms of third and higher order in $(x_1 - x_0)$ and $(z_1 - z_0)$ have been omitted. Kolsky proposed solving this overdetermined system of equations for $\frac{\partial P}{\partial x}$ and $\frac{\partial P}{\partial z}$ by first solving for $(P_1 - P_3)$ and $(P_2 - P_4)$, obtaining the two equations

$$(P_1 - P_3) = \frac{\partial P}{\partial x}(x_1 - x_3) + \frac{\partial P}{\partial z}(z_1 - z_3)$$

$$+ \frac{\partial^2 P}{\partial x^2}(x_1 - x_3)\delta_{x13} + \frac{\partial^2 P}{\partial z^2}(z_1 - z_3)\delta_{z13}$$

$$+ \frac{1}{2}\frac{\partial^2 P}{\partial x \partial z}\left[(x_1 - x_3)\delta_{z13} + (z_1 - z_3)\delta_{x13}\right] + \cdots$$

$$(P_2 - P_4) = \frac{\partial P}{\partial x}(x_2 - x_4) + \frac{\partial P}{\partial z}(z_2 - z_4)$$

$$+ \frac{\partial^2 P}{\partial x^2}(x_2 - x_4)\delta_{x24} + \frac{\partial^2 P}{\partial z^2}(z_2 - z_4)\delta_{z24}$$

$$+ \frac{1}{2}\frac{\partial^2 P}{\partial x \partial z}\left[(x_2 - x_4)\delta_{z24} - (z_2 - z_4)\delta_{x24}\right] + \cdots$$

where $\delta_{x13} = \frac{1}{2}(x_1 + x_2) - x_0$, etc. are measures of the assymmetry of the mesh. Omitted terms are of second and higher order in the mesh size $(x_1 - x_3)$, etc. Providing the mesh size is

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small, these higher order terms are negligible compared to the terms retained above. The above equations may now be solved for the gradients

$$a_x = -\frac{1}{\rho}\frac{\partial P}{\partial x} = -\frac{1}{2A\rho}\left\{(P_2-P_4)(z_1-z_3)-(P_1-P_3)(z_2-z_4)\right\} + R_x$$

3.11

$$a_z = -\frac{1}{\rho}\frac{\partial P}{\partial x} = \frac{1}{2A\rho}\left\{(P_2-P_4)(x_1-x_3)-(P_1-P_3)(x_2-x_4)\right\} + R_z$$

where

$$A = \frac{1}{2}\left\{(z_1-z_3)(x_2-x_4)-(x_1-x_3)(z_2-z_4)\right\}$$

It is seen that A represents the area of the quadrilateral 1 2 3 4.

The remainder terms R_x and R_z involve products of the mesh size and the δ's (e.g., $(x_1 - x_3)\,\delta_{x,3}$, etc.). If the mesh is nearly symmetric, these terms are negligible compared to the terms which have been retained. It is clear that the error terms vanish for an undistorted mesh, but become progressively larger as the mesh distorts.

Equations 3.9 require coordinates of the centroids of quadrilateral 1, 2, 3, 4. Kolsky simply used the approximate equation 3.5, obtaining the final equations

$$a_x = \frac{1}{8(A\rho)}\left\{(P_2-P_4)(z_c-z_A+z_B-z_D+z_F-z_H)\right.$$
$$\left.-(P_1-P_3)(z_c-z_A+z_D-z_B+z_G-z_E)\right\}$$

3.12

$$a_z = \frac{-1}{8(A\rho)}\left\{(P_2-P_4)(x_c-x_A+x_B-x_D+x_F-x_H)\right.$$
$$\left.-(P_1-P_3)(x_c-x_A+x_D-x_B+x_G-x_E)\right\}$$

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There are two possibilities for representing the denominator $(A\rho)$ in equation 3.12 in a simple form. Kolsky used[1]

$$(A\rho) = \frac{1}{4}\left(A_1\rho_1 + A_2\rho_2 + A_3\rho_3 + A_4\rho_4 \right) \qquad 3.13$$

A second expression follows from equation 3.3 for the cylindrical case

$$(A\rho) = \frac{1}{4}\left(m_1 + m_2 + m_3 + m_4 \right)/(x_o)^{\alpha-1} \qquad 3.14$$

where x_o is used as an approximation to the centroid of the quadrilateral 1 2 3 4. Equation 3.7 is used for the m's. For certain serious distortions this may lead to considerable error. For the rectangular case, equation 3.14 is equivalent to equation 3.13.

It may be noted parenthetically that the same results are achieved by starting with the alternate form of the momentum equation (equation 2.13), as may be expected. The Lagrangian pressure gradients may be represented by[2,3]

$$\frac{\partial P}{\partial X} = \frac{1}{\Delta X}\left(\frac{P_2 + P_1}{2} - \frac{P_3 + P_4}{2} \right) \qquad 3.15$$

$$\frac{\partial P}{\partial Z} = \frac{1}{\Delta Z}\left(\frac{P_1 + P_4}{2} - \frac{P_2 + P_3}{2} \right)$$

Inserting these together with equations 3.8 into equations 2.13 and simplifying,

$$a_Y = \frac{-(x/X)^{\alpha-1}}{2\rho_o \Delta X \Delta Z}\left\{ (P_2 - P_4)(z_1 - z_3) - (P_1 - P_3)(z_2 - z_4) \right\}$$

$$\qquad 3.16$$

$$a_Z = \frac{(x/X)^{\alpha-1}}{2\rho_o \Delta X \Delta Z}\left\{ (P_2 - P_4)(x_1 - x_3) - (P_1 - P_3)(x_2 - x_4) \right\}$$

With the aid of equations 2.3 and 3.9, (the latter written for quadrilateral 1 2 3 4), it is seen that the above equations 3.16 are exactly equivalent to the previous result, equations 3.11.

3.2.2 "Midpoint" Method
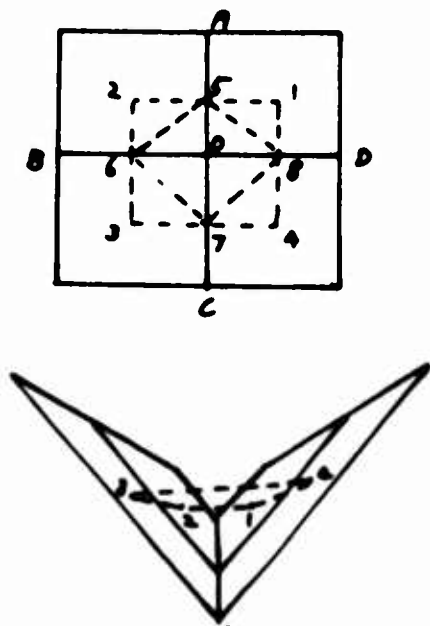
Amurud and Orr[4] noted that Kolsky's scheme led to reversal of signs of the accelerations when the mesh became sufficiently distorted so that quadrilateral 1 2 3 4 became inverted. They proposed applying Taylor's theorem between points 0-5, 0-6, 0-7 0-8 as shown, in conjunction with a test and approximate correction procedure to prevent inversion of quadrilateral 5 6 7 8.

Substituting subscripts 5, 6, 7, 8 for subscripts 1, 2, 3, 4 in equations 3.11 and writing

$$P_5 = \tfrac{1}{2}\left(P_1 + P_2\right) \qquad \text{etc.}$$

$$x_5 = \tfrac{1}{2}\left(x_A + x_0\right) \qquad \text{etc.}$$
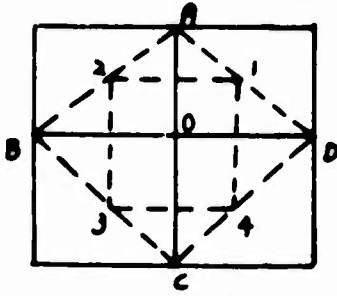
the following equations result

$$a_x = \frac{1}{8(A\rho)}\left\{(P_1 - P_3)(z_A - z_c + z_B - z_D)\right.$$

$$\left. -(P_2 - P_4)(z_A - z_c + z_D - z_B)\right\}$$

$$a_z = \frac{-1}{8(A\rho)}\left\{(P_1 - P_3)(x_A - x_c + x_B - x_D)\right.$$

$$\left. -(P_2 - P_4)(x_A - x_c + x_D - x_B)\right\}$$

3.17

The same expressions may be used for $(A\rho)$ as before (equations 3.13 and 3.14).

3.2.3 Green's Transformation

A different approach to the problem of finding pressure gradients follows from Green's Transformation[5,6] In two dimensions

$$\oint_{\mathcal{S}} P n_i \, ds = \int_A P_{,i} \, da \qquad 3.18$$

where n_i is the outward normal vector to the circuit $\mathcal{S}$ enclosing the area A, and the comma denotes covariant differentiation. In component form, we are led to the two equations

$$\oint_{\mathcal{S}} p \, dz = \int \frac{\partial P}{\partial x} \, dA = \left(\frac{\partial P}{\partial x} \right)_{AVE} \cdot A$$

$$-\oint_{\mathcal{S}} p \, dx = \int \frac{\partial P}{\partial x} \, dA = \left(\frac{\partial P}{\partial z} \right)_{AVE} \cdot A$$

$$3.19$$

Choosing the circuit A B C D, and considering the pressure on side A B to be given by its average value p_2 etc.,

$$a_x = -\frac{1}{\rho} \frac{\partial P}{\partial x} = \frac{1}{2(A\rho)} \left\{ P_1 (z_A - z_D) + P_2 (z_B - z_A) + P_3 (z_C - z_B) + P_4 (z_D - z_C) \right\}$$

$$3.20$$

$$a_z = -\frac{1}{\rho} \frac{\partial P}{\partial z} = \frac{-1}{2(A\rho)} \left\{ P_1 (x_A - x_D) + P_2 (x_B - x_A) + P_3 (x_C - x_B) + P_4 (x_D - x_C) \right\}$$

where A is one half the area of the quadrilateral A B C D. A reasonable approximation to the denominator is given by equation 3.13 or equation 3.14. For irregular distortions, a better but much lengthier expression would be

$$A\rho = \frac{1}{2} \left(A_1' \rho_1 + A_2' \rho_2 + A_3' \rho_3 + A_4' \rho_4 \right) \qquad 3.21$$

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where A_1' is the area of triangle A O D etc.

Variations of equations 3.20 suggests themselves. Instead of representing ($A\rho$) by equation 3.21, we write

$$a_x = \left\{ \frac{P_1 (z_A - z_D)}{2 A_1 \rho_1} + \frac{P_2 (z_B - z_A)}{2 A_2 \rho_2} + \frac{P_3 (z_C - z_B)}{2 A_3 \rho_3} + \frac{P_4 (z_D - z_C)}{2 A_4 \rho_4} \right\}$$

3.22

$$a_z = -\left\{ \frac{P_1 (x_A - x_D)}{2 A_1 \rho_1} + \frac{P_2 (x_B - x_A)}{2 A_2 \rho_2} + \frac{P_3 (x_C - x_B)}{2 A_3 \rho_3} + \frac{P_4 (x_D - x_C)}{2 A_4 \rho_4} \right\}$$

where A_1 etc. are the areas of quadrilaterals A O D H etc. In these equations the contribution of each mesh to the acceleration is independent of the other meshes. We can also use equation 3.3 to write

$$A_1 \rho_1 = \frac{m_1}{(\bar{x}_1)^{d-1}}$$

3.23

etc., where we use equation 3.5 for $\bar{x}_1$, in each of the above terms. A further variation is to write

$$A_1 \rho_1 = 2 A_1' \rho_1$$

3.24

etc., where A_1' is the area of triangle A O D, in each of the above terms.

It may be noted parenthetically that if circuit 1 2 3 4 is chosen, the results obtained previously by means of Taylor's Theorem are obtained. The average pressure on side 1 2 can be written $\frac{1}{2}(P_1 + P_2)$. Thus, applying equations 3.19 to the circuit 1 2 3 4,

$$a_x = \frac{1}{2 A \rho} \left\{ (P_2 + P_1)(z_2 - z_1) + (P_3 + P_2)(z_3 - z_2) \right.$$
$$\left. + (P_4 + P_3)(z_4 - z_3) + (P_1 + P_4)(z_1 - z_4) \right\}$$

3.25

$$a_z = \frac{-1}{2 A \rho} \left\{ (P_2 + P_1)(x_2 - x_1) + (P_3 + P_2)(x_3 - x_2) \right.$$
$$\left. + (P_4 + P_3)(x_4 - x_3) + (P_1 + P_4)(x_1 - x_4) \right\}$$

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where A is the area of quadrilateral 1 2 3 4. Upon simplification and interpolation of x and z these reduce to equations 3.12.

Green's Transformation has also been used to obtain expressions of the gradients in a triangular mesh.[7] Triangular meshes are generally found to be anisotropic and are not considered here.

3.2.4 "Force Gradients" Method
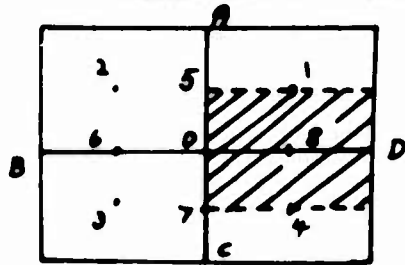
An expression for the gradients in use at L.A.S.L.[8] may be derived in several ways. For the shaded zone, Lagrangian gradients may be expressed as

$$\left(\frac{\partial P}{\partial x}\right)_e = \frac{P_1 - P_4}{X_1 - X_4} \qquad \left(\frac{\partial z}{\partial z}\right)_e = \frac{z_D - z_0}{Z_D - Z_0}$$

Writing similar expressions for the zone 2 B 3 0 on the opposite side of 0, and interpolating, the x gradient at 0 can be written (from equation 2.13)

$$a_x = -\frac{1}{2\rho_0} \left\{ \frac{(P_1 - P_4)(z_D - z_0)}{(X_1 - X_4)(Z_D - Z_0)} \left(\frac{\bar{x}}{\bar{X}}\right)_e^{\alpha-1} + \frac{(P_2 - P_3)(z_0 - z_B)}{(X_2 - X_3)(Z_0 - Z_B)} \left(\frac{\bar{x}}{\bar{X}}\right)_6^{\alpha-1} \right.$$

$$\left. - \frac{(P_1 - P_2)(z_A - z_0)}{(Z_1 - Z_2)(X_A - X_0)} \left(\frac{\bar{x}}{\bar{X}}\right)_5^{\alpha-1} - \frac{(P_4 - P_3)(z_0 - z_c)}{(Z_4 - Z_3)(X_0 - X_c)} \left(\frac{\bar{x}}{\bar{X}}\right)_7^{\alpha-1} \right\}$$

3.26

with a similar expression for a_z. Two ways of representing the denominators of the terms above follow from the mass equation. We note that the denominator of the first term $(X_1 - X_4)(Z_0 - Z_0)$ represents the undeformed area of the shaded rectangle, denoted by $(\ )_e$. Using equation 3.4

$$\rho_0 (X_1 - X_4)(Z_D - Z_0)(\bar{x})^{\alpha-1} = m_e = \frac{1}{2}(m_1 + m_4)$$

18

Proceeding in this way, the accelerations become

$$a_x = -\frac{(P_1 - P_4)(z_D - z_o)}{(m_1 + m_4)}\left(\frac{x_D + x_o}{2}\right)^{\alpha-1} - \frac{(P_2 - P_3)(z_o - z_B)}{(m_2 + m_3)}\left(\frac{x_o + x_B}{2}\right)^{\alpha-1}$$

$$+ \frac{(P_1 - P_2)(z_A - z_o)}{(m_1 + m_2)}\left(\frac{x_A + x_o}{2}\right)^{\alpha-1} + \frac{(P_4 - P_3)(z_o - z_c)}{(m_4 + m_3)}\left(\frac{x_o + x_c}{2}\right)^{\alpha-1}$$

<div align="right">3.27</div>

$$a_z = \frac{(P_1 - P_4)(x_D - x_o)}{(m_1 + m_4)}\left(\frac{x_D + x_o}{2}\right)^{\alpha-1} + \frac{(P_2 - P_3)(x_o - x_B)}{(m_2 + m_3)}\left(\frac{x_o + x_B}{2}\right)^{\alpha-1}$$

$$- \frac{(P_1 - P_2)(x_A - x_o)}{(m_1 + m_2)}\left(\frac{x_A + x_o}{2}\right)^{\alpha-1} - \frac{(P_4 - P_3)(x_o - x_c)}{(m_4 + m_3)}\left(\frac{x_o + x_c}{2}\right)^{\alpha-1}$$

where we have simply approximated $\bar{x}_\beta = \frac{1}{2}\left(x_D + x_o\right)$ etc.

Alternatively, using equation 3.3 these equations can be put into the form

$$a_x = -\frac{(P_1 - P_4)(z_D - z_o)}{P_1 A_1 + P_4 A_4} - \frac{(P_2 - P_3)(z_o - z_B)}{P_2 A_2 + P_3 A_3}$$

$$+ \frac{(P_1 - P_2)(z_A - z_o)}{P_1 A_1 + P_2 A_2} + \frac{(P_4 - P_3)(z_o - z_c)}{P_4 A_4 + P_3 A_3}$$

<div align="right">3.28</div>

$$a_z = \frac{(P_1 - P_4)(x_D - x_o)}{P_1 A_1 + P_4 A_4} + \frac{(P_2 - P_3)(x_o - x_B)}{P_2 A_2 + P_3 A_3}$$

$$- \frac{(P_1 - P_2)(x_A - x_o)}{P_1 A_1 + P_2 A_2} - \frac{(P_4 - P_3)(x_o - x_c)}{P_4 A_4 + P_3 A_3}$$

19

The two approximations made in the denominators of equations 3.27 and 3.28 are analogous to the approximations made in equations 3.14 and 3.13.

The above equations (3.27 or 3.28) lead to difficulties for certain serious distortions in which one or more of the segments OA, OB, OC, or OD approach zero length. More complex equations, apparently derived on a similar basis, but involving multiple interpolations to overcome this drawback, have been reported.[9]

3.2.5 Virtual Work Method
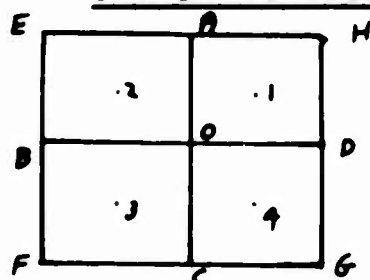
Goad[10] proposed a method of obtaining the apparent force, and hence the acceleration, on a mass point located at 0 by the principle of virtual work. Suppose that the point 0 is displaced by an infinitesimal vector displacement δs^k Work is done on the surrounding four cells, and the energy of the system is modified by an increment δE given by

$$\delta E = \sum_{i=1}^{4} \left(p \, \delta s^k \, v_{,k} \right)_i$$

where v is the cell volume, and the comma denotes covariant differentiation. Thus a force F_k acts at 0 given by

$$\delta E = F_k \, \delta s^k$$

Thus

$$F_k = \sum_{i=1}^{4} \left(p \, v_{,k} \right)_i$$

and the acceleration at 0 is therefore

$$a_k = \frac{F_k}{m} = \frac{1}{m} \sum_{i=1}^{4} \left(p \, v_{,k} \right)_i$$

where m is the mass which is thought of as being concentrated at point 0.

Using the second method of finding the volume of a mesh, (Subsection 3.1) for mesh 1 we have within a factor $(2\pi)^{\alpha - 1}$)

$$v_1 = \left\{ A_L \left(\bar{x}_L \right)^{\alpha - 1} + A_u \left(\bar{x}_u \right)^{\alpha - 1} \right\}$$

20

where A_L, $\bar{x}_L$ etc. are given following equation 3.6. To find the derivatives of ν, we consider x_o, z_o variable with the other cell vertices held fixed, and obtain for the x direction for cell 1

$$\left(p\, \nu_{,x} \right)_1 = \frac{1}{2}\, P_1 \left\{ \left(\frac{x_o + x_b + x_A}{3} \right)^{\alpha-1} (z_A - z_b) \right.$$

$$\left. + \frac{1}{3}(\alpha-1)\left[(z_b - z_o)(x_A - x_o) - (z_A - z_o)(x_b - x_o) \right] \right\}$$

while for the z direction for cell 1

$$\left(p\, \nu_{,z} \right)_1 = \frac{1}{2}\, P_1 \left\{ \left(\frac{x_o + x_b + x_A}{3} \right)^{\alpha-1} (x_b - x_A) \right\}$$

The mass m associated with point 0 may be taken to be (within a factor $(2\pi)^{\alpha-1}$)

$$m = \frac{1}{4} \left(m_1 + m_2 + m_3 + m_4 \right) \qquad\qquad 3.29$$

where m_1 etc. are given by equation 3.7.

Summing terms for all four meshes

$$a_x = \frac{1}{2m} \left\{ P_1 \left[\left(\frac{x_o + x_b + x_A}{3} \right)^{\alpha-1} (z_A - z_b) + \frac{\alpha-1}{3}\left[(z_b - z_o)(x_A - x_o) - (z_A - z_o)(x_b - x_o) \right] \right] \right.$$

$$+ P_2 \left[\left(\frac{x_o + x_A + x_b}{3} \right)^{\alpha-1} (z_b - z_A) + \frac{\alpha-1}{3}\left[(z_A - z_o)(x_b - x_o) - (z_b - z_o)(x_A - x_o) \right] \right]$$

$$+ P_3 \left[\left(\frac{x_o + x_b + x_c}{3} \right)^{\alpha-1} (z_c - z_b) + \frac{\alpha-1}{3}\left[(z_b - z_o)(x_c - x_o) - (z_c - z_o)(x_b - x_o) \right] \right]$$

$$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad 3.30$$

$$\left. + P_4 \left[\left(\frac{x_o + x_c + x_b}{3} \right)^{\alpha-1} (z_b - z_c) + \frac{\alpha-1}{3}\left[(z_c - z_o)(x_b - x_o) - (z_b - z_o)(x_c - x_o) \right] \right] \right\}$$

$$a_z = \frac{-1}{2m} \left\{ P_1 \left(\frac{x_o + x_b + x_A}{3} \right)^{\alpha-1} (x_A - x_b) + P_2 \left(\frac{x_o + x_A + x_b}{3} \right)^{\alpha-1} (x_b - x_A) \right.$$

$$\left. + P_3 \left(\frac{x_o + x_b + x_c}{3} \right)^{\alpha-1} (x_c - x_b) + P_4 \left(\frac{x_o + x_c + x_o}{3} \right)^{\alpha-1} (x_b - x_c) \right\}$$

For the rectangular case, $\alpha = 1$, and the equations reduce identically to these obtained by Green's Transformation (equations 3.20).

SECTION IV

RESULTS AND DISCUSSION

Results of a number of calculations are given in this section. Both the analytical and finite-difference equations were programmed for computation on an IBM 7094 Computer. Results are shown in the figures, where results of the various finite difference equations are labeled as follows.

1. Taylor Expansion   Eq. 3.12 with Eq. 3.13
2. Taylor Expansion   Eq. 3.12 with Eq. 3.14
3. Midpoint Method   Eq. 3.17 with Eq. 3.13
4. Midpoint Method   Eq. 3.17 with Eq. 3.14
5. Greens Transformation   Eq. 3.20 with Eq. 3.13
6. Greens Transformation   Eq. 3.20 with Eq. 3.14
7. Greens Transformation   Eq. 3.22
8. Greens Transformation   Eq. 3.22 with Eq. 3.23
9. Greens Transformation   Eq. 3.20 with Eq. 3.21
10. Greens Transformation   Eq. 3.22 with Eq. 3.24
11. Force Gradients   Eq. 3.28
12. Force Gradients   Eq. 3.27
13. Virtual Work   Eq. 3.30

In each case the accelerations a^x and a^z were converted to magnitude a and direction θ by

$$a = \sqrt{(a^x)^2 + (a^z)^2}$$

$$\theta = \arctan \frac{a^x}{a^z}$$

4.1

and percentage errors in magnitude, and angular errors in direction compared to the true magnitude and direction were found.

It is difficult to present results to illustrate the growth of the error as a function of some measure of deformation. Since the equation of state (equation 2.9) was nonlinear, the

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results, expressed as a percentage of true acceleration, would be affected appreciably by the addition of a uniform (hydrostatic) compression. Moreover, in the cylindrically symmetric case ($\alpha = 2$), the results would be heavily affected by a uniform translation in the radial (x) direction. In order to eliminate these effects to some extent the following procedure was adopted. The quadratic coefficients (c) were adjusted incrementally in some arbitrary manner. The diagonal linear coefficients (d_{11}, d_{33}) were then given values such that the mesh with largest area was reduced to the area it had before deformation. Finally the coefficient b_1 was adjusted so that the radius of the mesh vertex with minimum radius was set equal to the minimum radius before deformation. This procedure did not eliminate the effects of uniform compression or radial translation, if indeed such would be desirable, but ensured that the effects of uniform compression or translation did not dominate.

It may be noted that if only c_{11}, d_{11} and b_1 are adjusted, then the deformation is one-dimensional, i.e., there is no deformation in the z direction. It is easily verified that for such a deformation all of the finite difference equations immediately reduce to the well known second order one-dimensional difference analog for $\alpha = 1$

$$a^2 = \frac{P_3 - P_1}{\frac{1}{2}\left\{ P_1(x_A - x_B) + P_3(x_B - x_C)\right\}}$$

4.2

where we note that $P_1 = P_2$, $P_3 = P_4$ etc. It is therefore possible to check the error of the one-dimensional difference analog directly.

Results are shown in Fig. 2, where the percentage error is plotted vs. the coefficient c_{11}. Deformed mesh shapes are also shown to give a physical picture of the deformation. It is quite clear that the error grows to very large proportions as the distortion becomes large.

Results of a number of calculations in which several
of the quadratic coefficients were varied incrementally are
shown in Fig. 3 through 8 (for $\alpha = 1$). In each case the next
increment in deformation coefficients led to inversion of one
or more meshes, i.e., one or more mesh areas became negative.
Errors below 1% were not considered significant. Deformed mesh
shapes are again shown to allow the deformation to be visualized.
The errors grow very rapidly as the deformation becomes extreme.
The difference in error of the various finite difference equa-
tions is, in most cases, unimportant compared to the magnitude
of the error. However, **results labeled 5-13 are generally**
somewhat better than these **labeled 1-4 (Taylor Expansion and**
Midpoint Method). One exception may be noted in Fig. 7 where
method 10 (Eq. 3.22 using Eq. 3.24) is much better than all the
others. In all cases the error in angle did not exceed a few
degrees for the most extreme deformations, and was quite neg-
ligible over most of the range.

Similar results for $\alpha = 2$ are shown in Fig. 9 through
16, the errors in both magnitude and angle being shown. Defor-
mations correspond to those in Fig. 3, 4, 5 and 7 respectively.
The errors in magnitude are generally smaller than the corre-
sponding errors for $\alpha = 1$. None of the errors approach zero
as the deformation is reduced. This may be traced to the ef-
fect of radial translation, and is not a serious concern. It
is clear from the results that no one finite difference equa-
tion is clearly superior, and errors of 20-30% in magnitude and
20-30 degrees in angle might be anticipated under certain con-
ditions with any of them.

While crossing of mass points could be observed by
suitable adjustment of the quadratic coefficients, this occurred,
for the combinations used above, during very severe distortions
where the error was extremely high. The effect of crossing of

mass points is somewhat more easily illustrated by choosing a different deformed mesh shape for which the true acceleration was not found. Several stages in crossing of mass points may be distinguished.

Normal

Re-entrant

Schizoid

Inverted Schizoid

Inverted
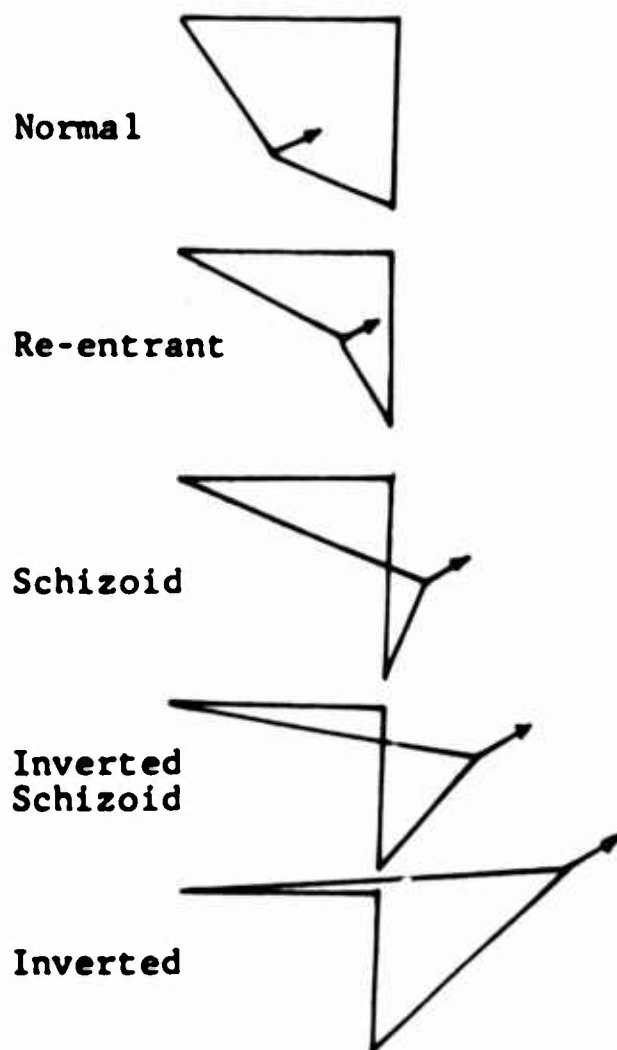
In a normal mesh, all included interior angles are less than 180°, as shown.

The first stage of crossing occurs when one included interior angle exceeds 180°. This may be termed a re-entrant mesh.

The second stage of crossing occurs when one mesh vertex crosses an opposite side. The mesh then takes the form of two triangles, one of which has a negative area. This may be termed a schizoid mesh.

If the deformation proceeds far enough, the net area of the mesh becomes negative. This may be termed an inverted mesh.

The effect of each stage was investigated by solving the finite difference equations for the mesh configurations shown in Fig. 17. Configuration (a) corresponded to a normal mesh. The acceleration was directed to the original position of the central vertex, for $\alpha = 1$, as might be expected. (For $\alpha = 2$, the net radial displacement of the centroids of the meshes leads to an acceleration directed in a slightly different direction).

In configuration (b) the upper left-hand mesh becomes

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re-entrant. All finite-difference equations gave the expected acceleration direction except 10 (Eq. 3.22 using Eq. 3.24) which showed an error near 180°. This reversal in acceleration would lead to an accentuation of the deformation, and hence instability. In configuration (c) the upper left-hand mesh became schizoid. Here both 9 (Eq. 3.20 using Eq. 3.21) and 10 (Eq. 3.22 using Eq. 3.24) showed an acceleration reversal, the other finite-difference equations giving the correct direction. In configuration (d) the upper left-hand mesh has become inverted. All equations gave an acceleration reversal. (This is traceable in part to the fact that the density in the inverted mesh becomes negative. The computer library routine for raising a number to a floating point exponent then gave a negative pressure, from equation 2.9, which was sufficiently large to outweigh the contributions of the negative pressures in the other expanded meshes.)

In assessing the results of the calculations presented in this report, it seems that none of the finite difference equations which were used are notably superior in accuracy. All except 9 and 10 (Eq. 3.20 using Eq. 3.21 and Eq. 3.22 using Eq. 3.24) showed no reversals in direction of the acceleration until at least one mesh area became negative. At this point all methods failed.

While the present calculations are hardly extensive enough to warrant drawing general conclusions, it does appear that any of the methods are equally satisfactory, provided a sufficiently small mesh size is chosen. It seems appropriate to choose the method which requires the least number of arithmetic steps for solution. Equations 3.20 seem most suitable for this reason.

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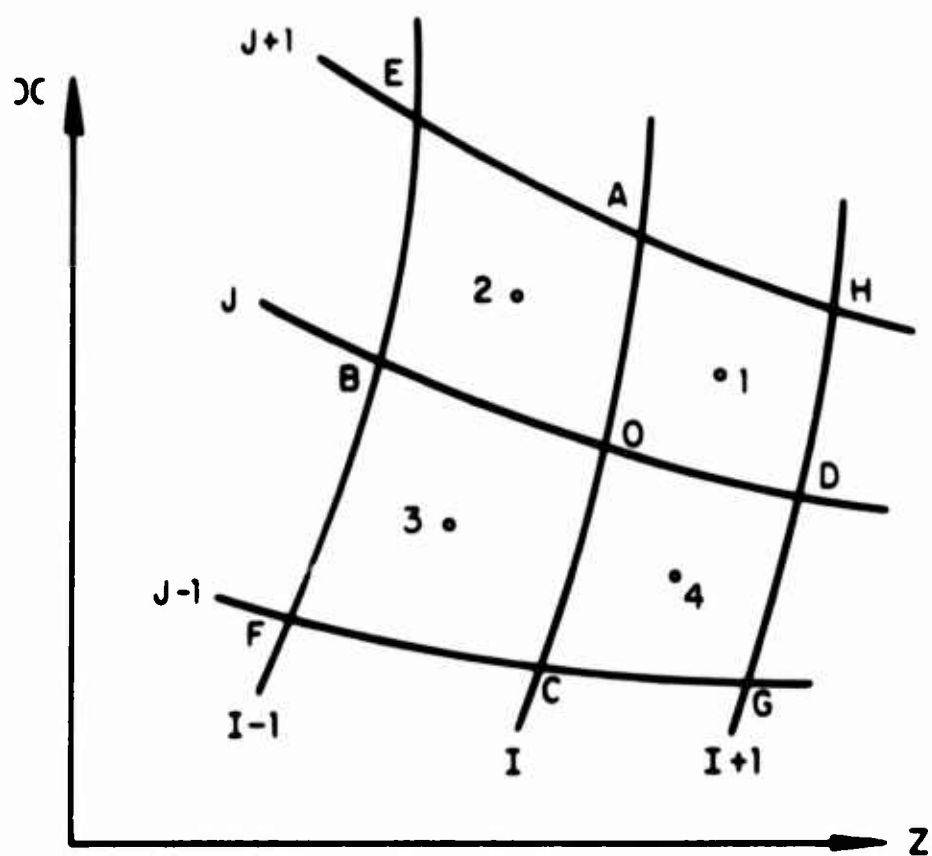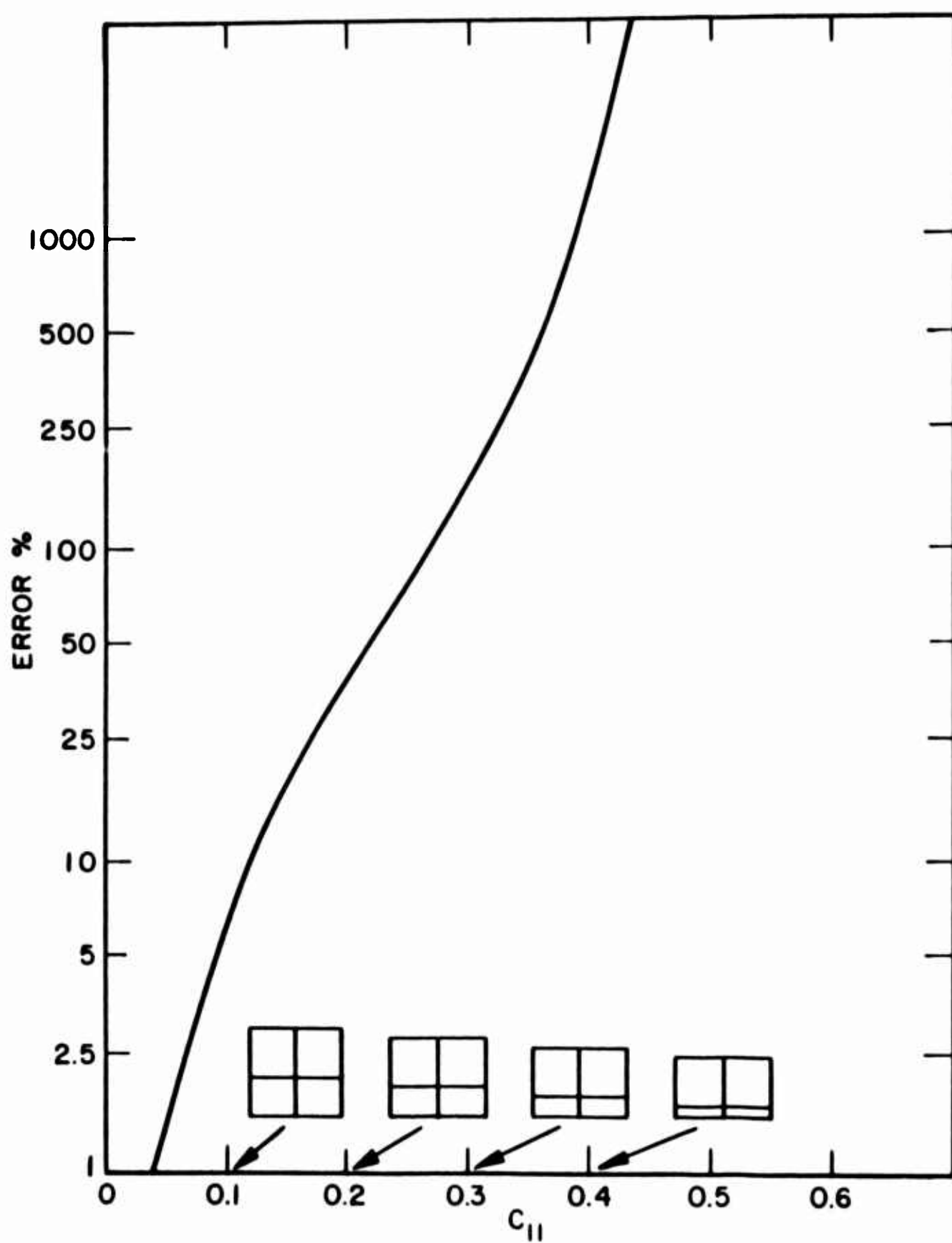
Figure 1   Finite Difference Mesh, Notation
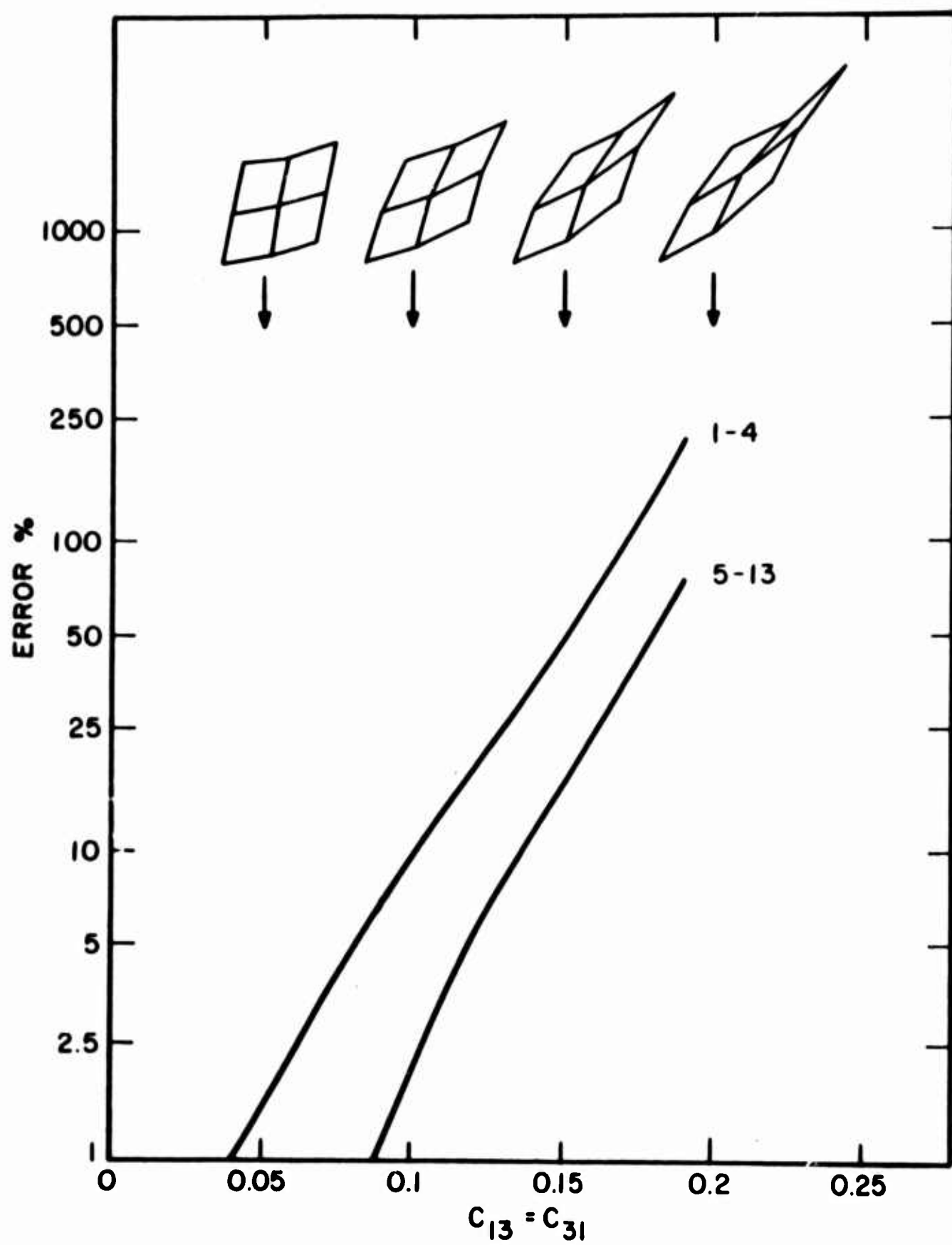
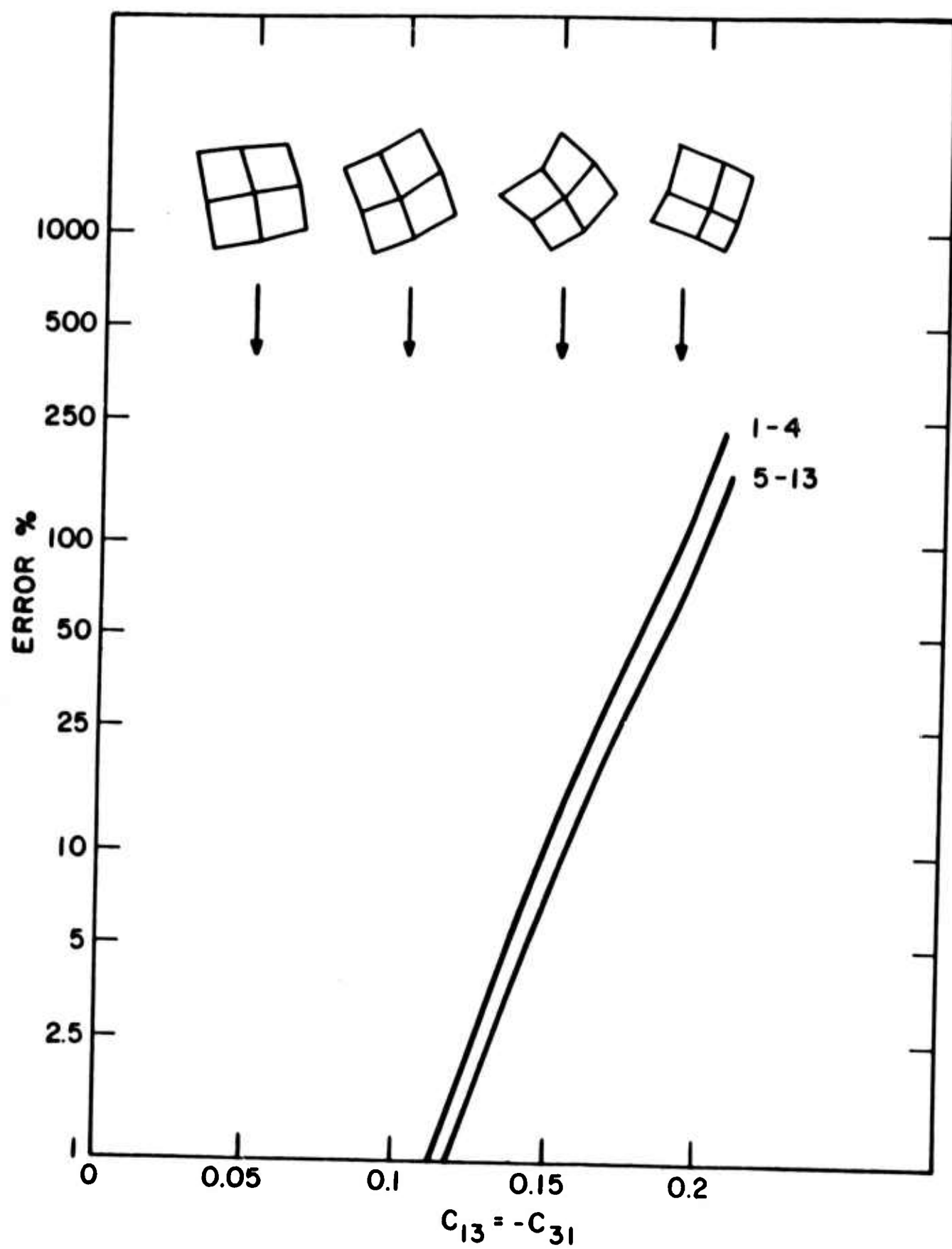Figure 2   One-Dimensional Differencing Error

Figure 3 Pure Shear, α - 1

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Figure 4   Pure Rotation, α = 1

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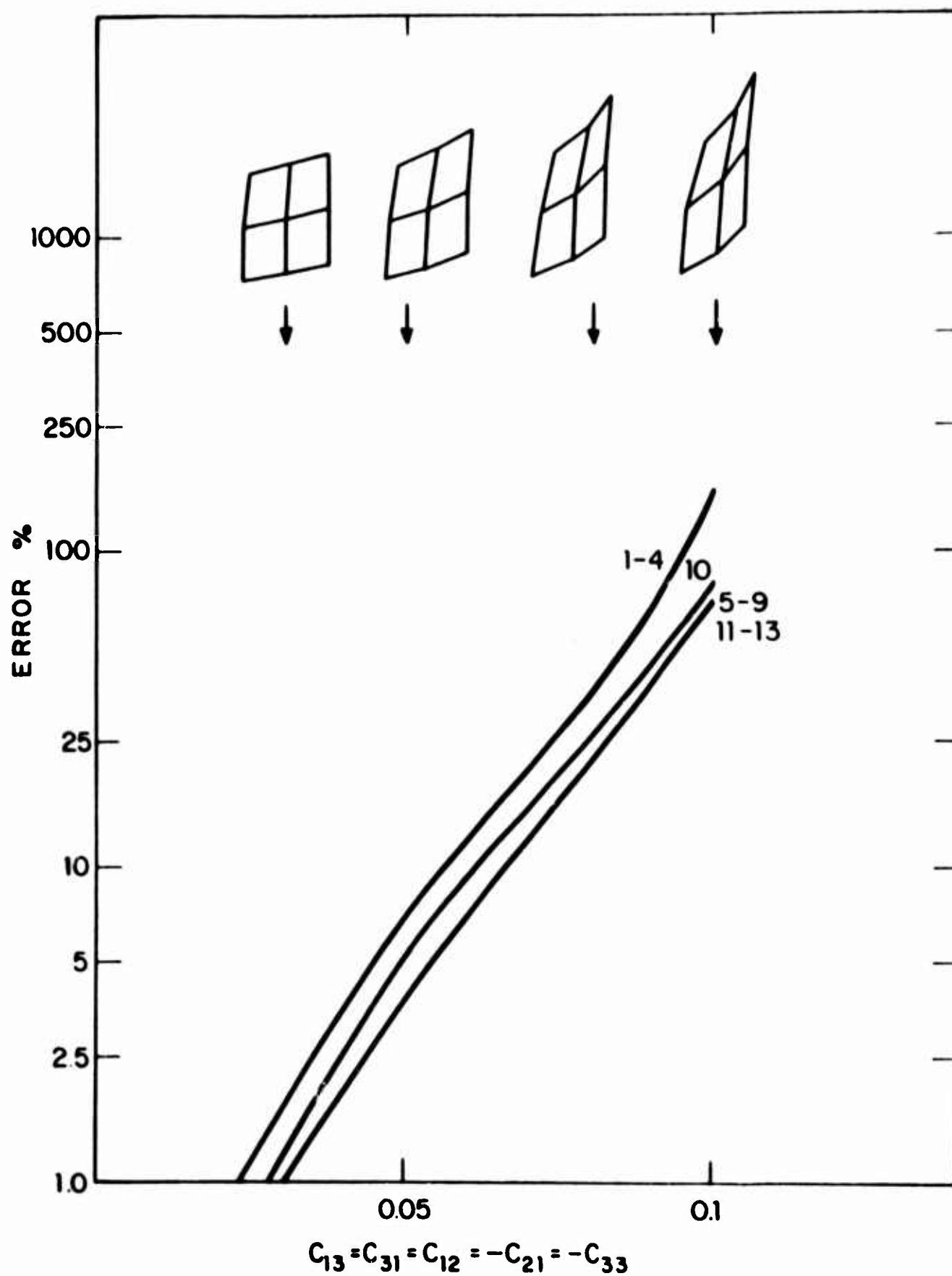
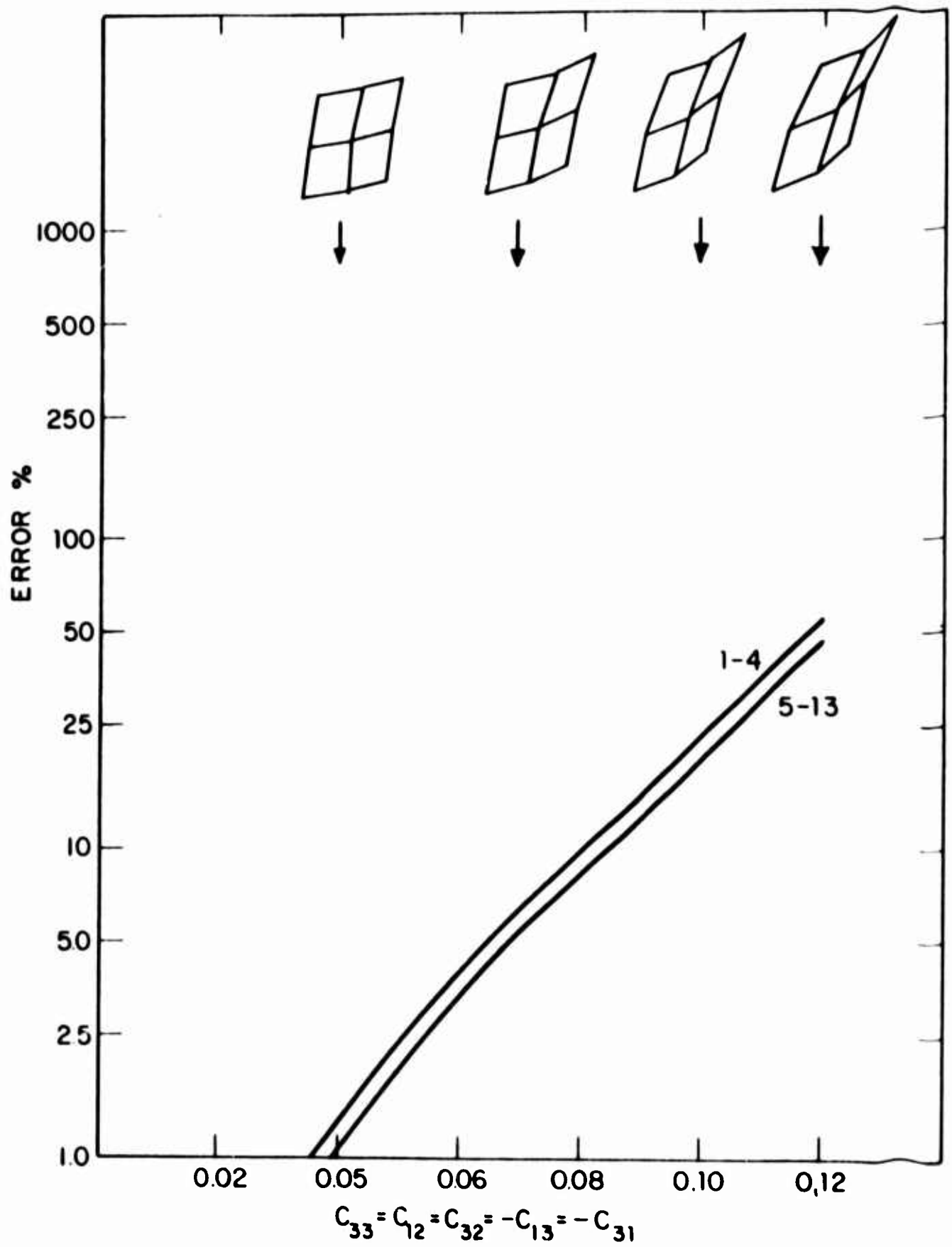Figure 5 Shear, Rotation and Compression, α = 1

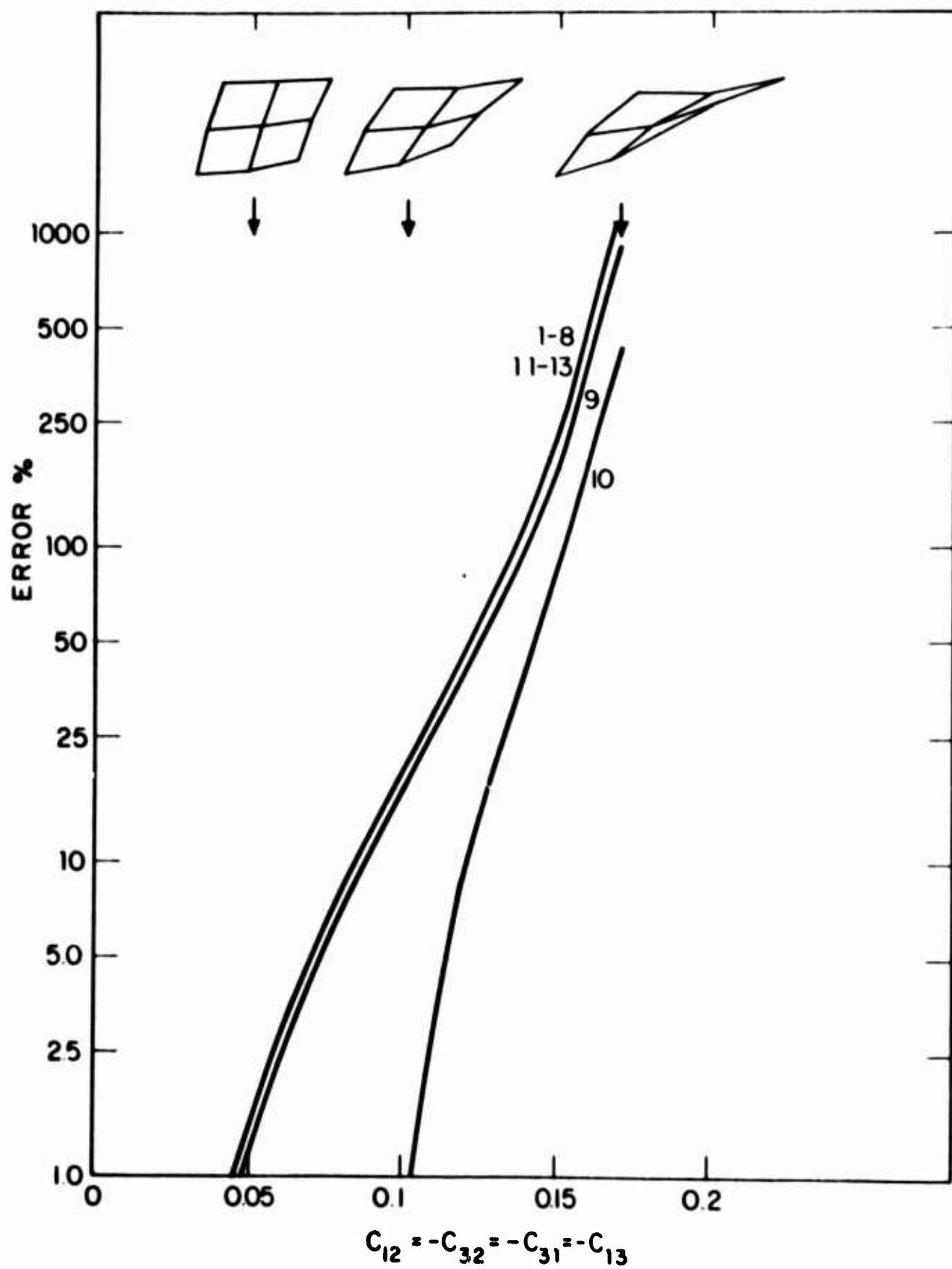Figure 6   Shear and Compression, $\alpha = 1$

35
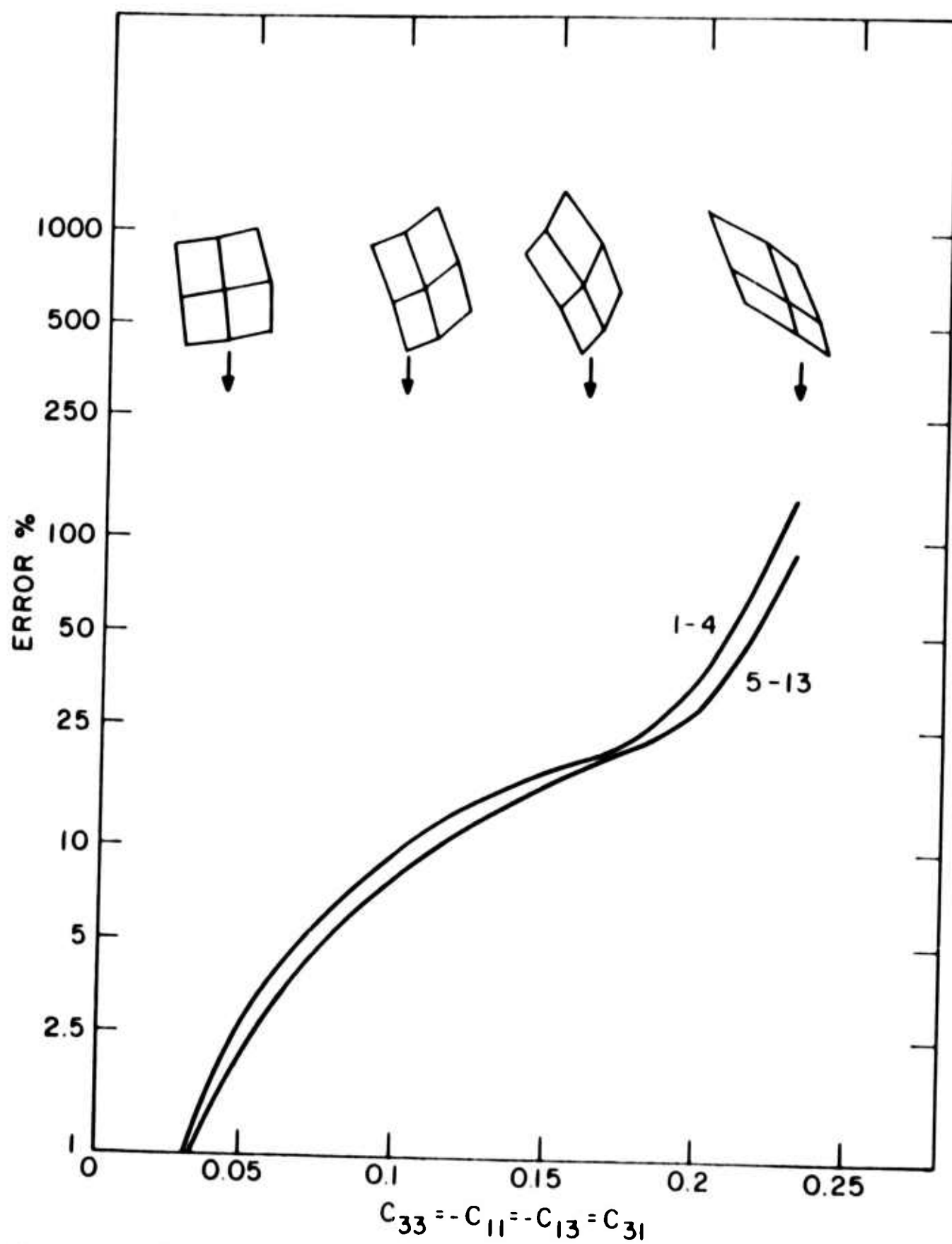
Figure 7 Shear and Rotation, $\alpha = 1$

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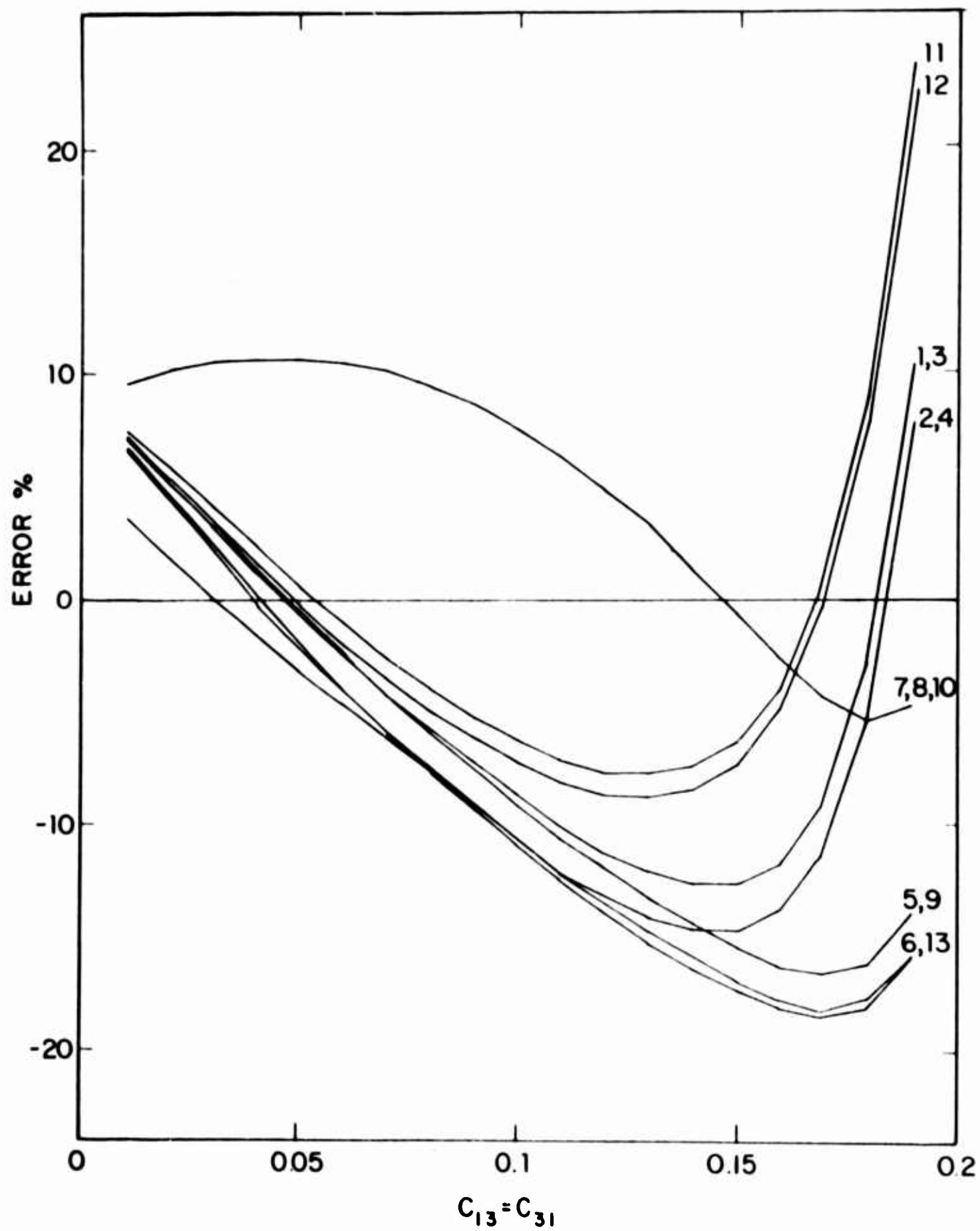Figure 8 Compression and Rotation, $\alpha = 1$

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Figure 9 Pure Shear, $\alpha = 2$ Magnitude Error

38
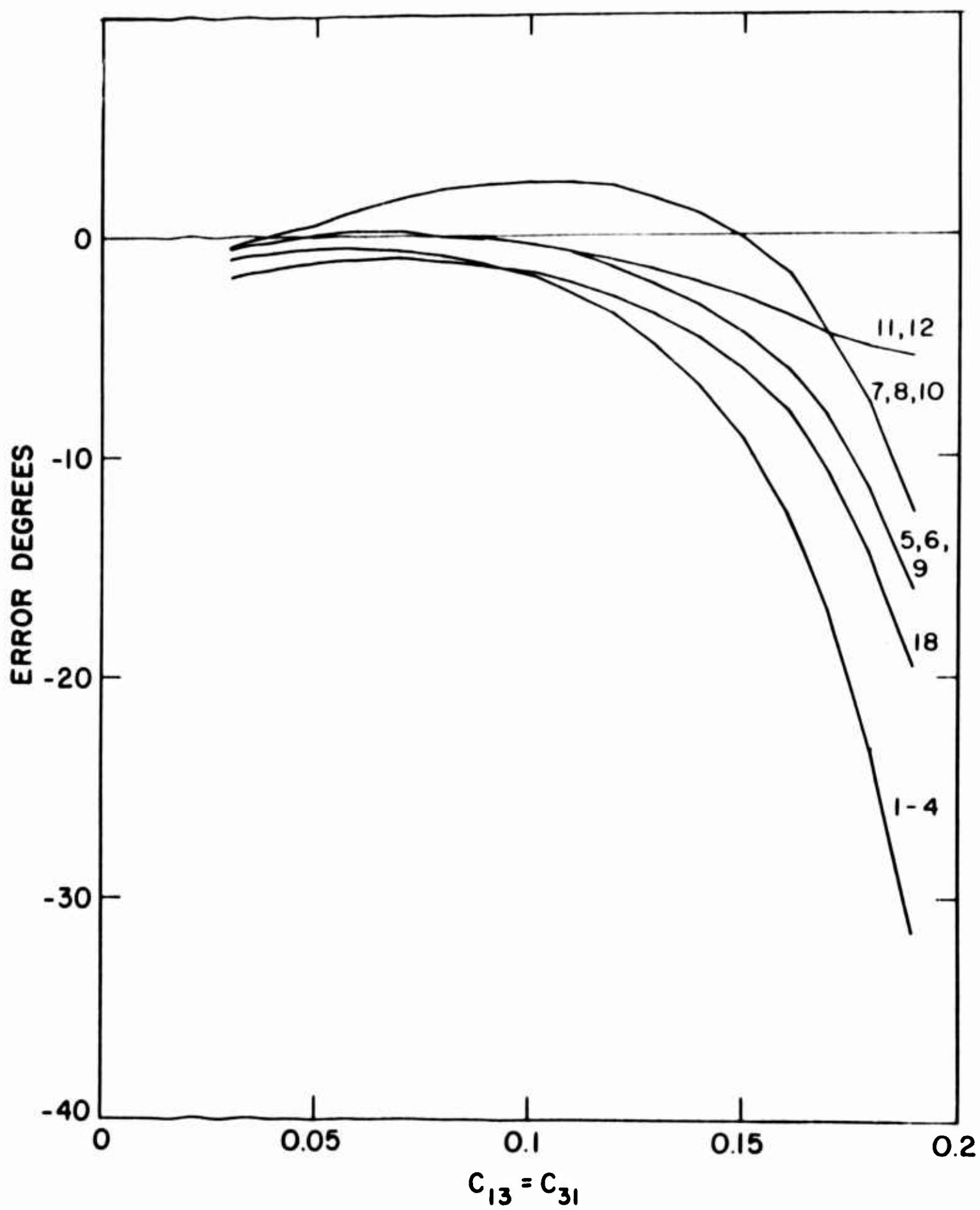
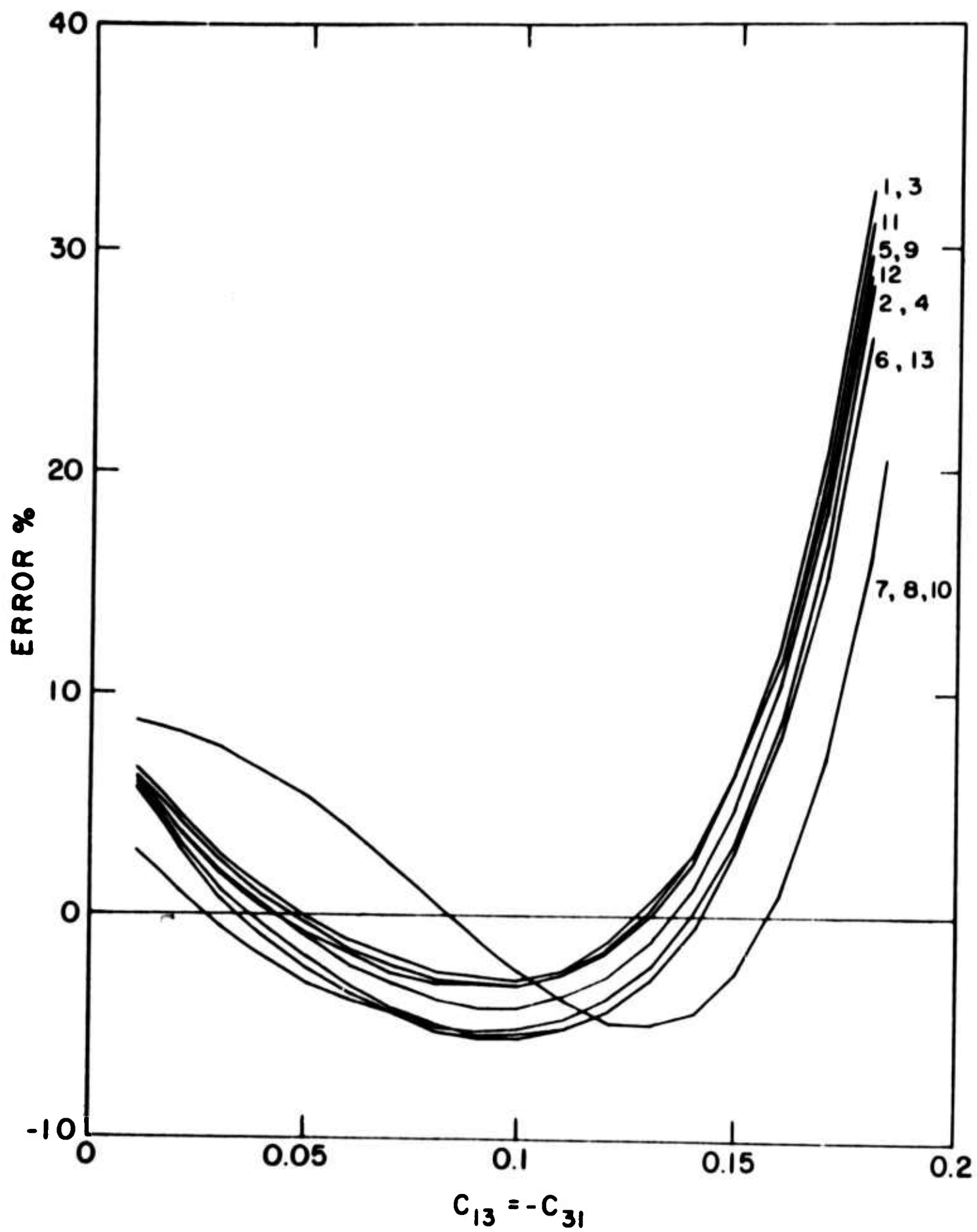Figure 10   Pure Shear, α = 2   Angular Error

Figure 11 Pure Rotation, $\alpha = 2$ Magnitude Error
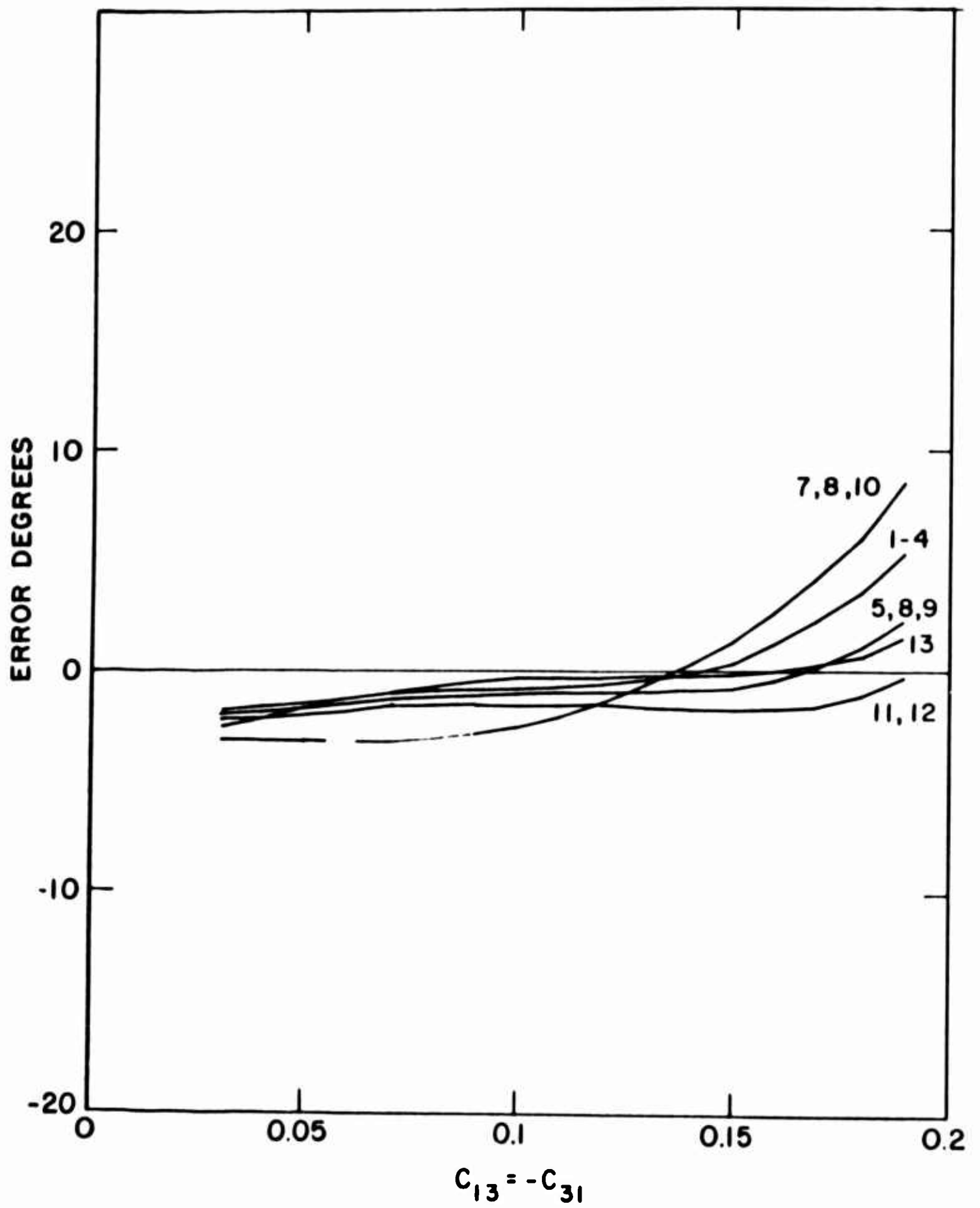
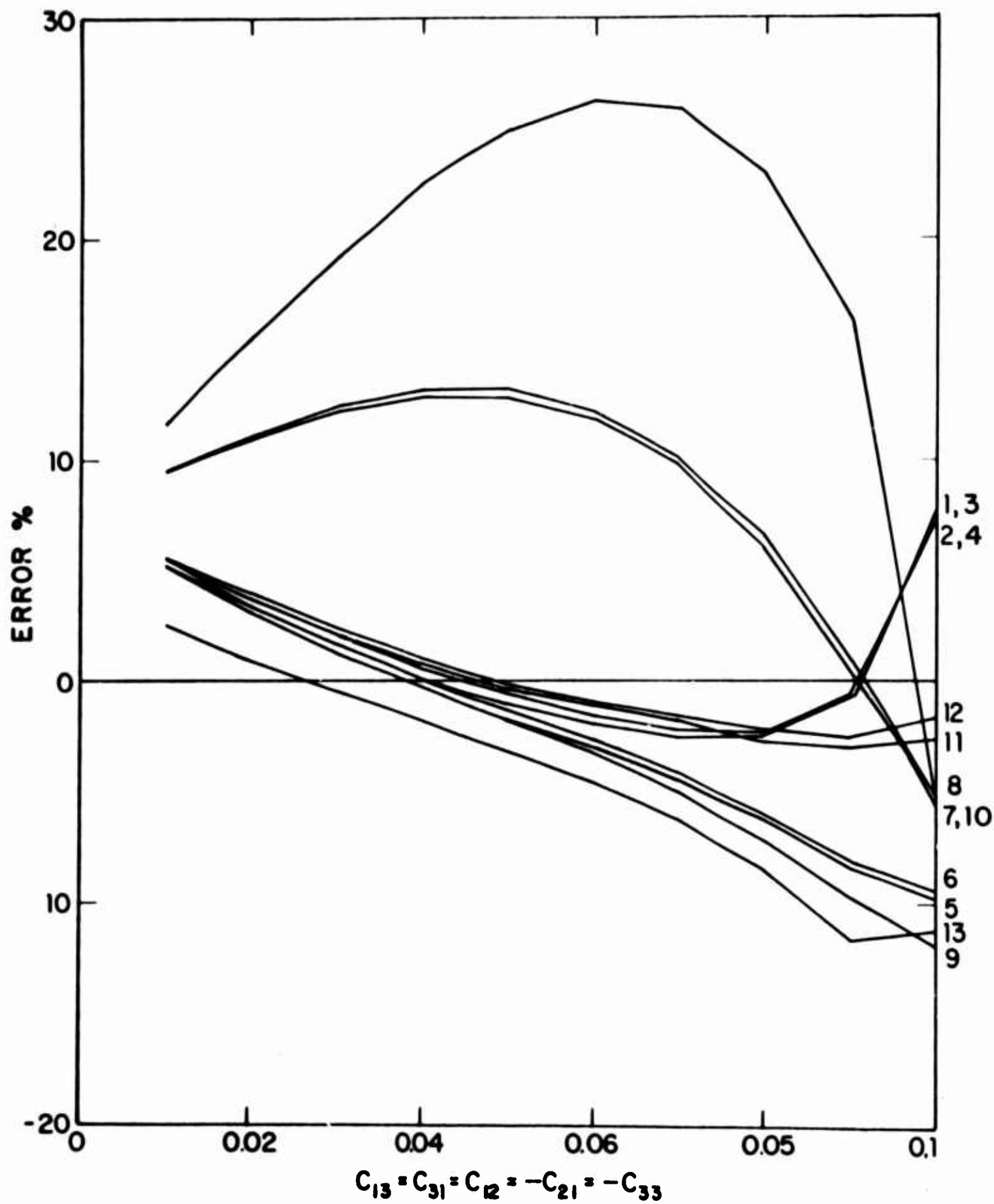Figure 12   Pure Rotation, $\alpha = 2$ Angular Error

Figure 13   Shear, Rotation and Compression, $\alpha = 2$ Magnitude Error
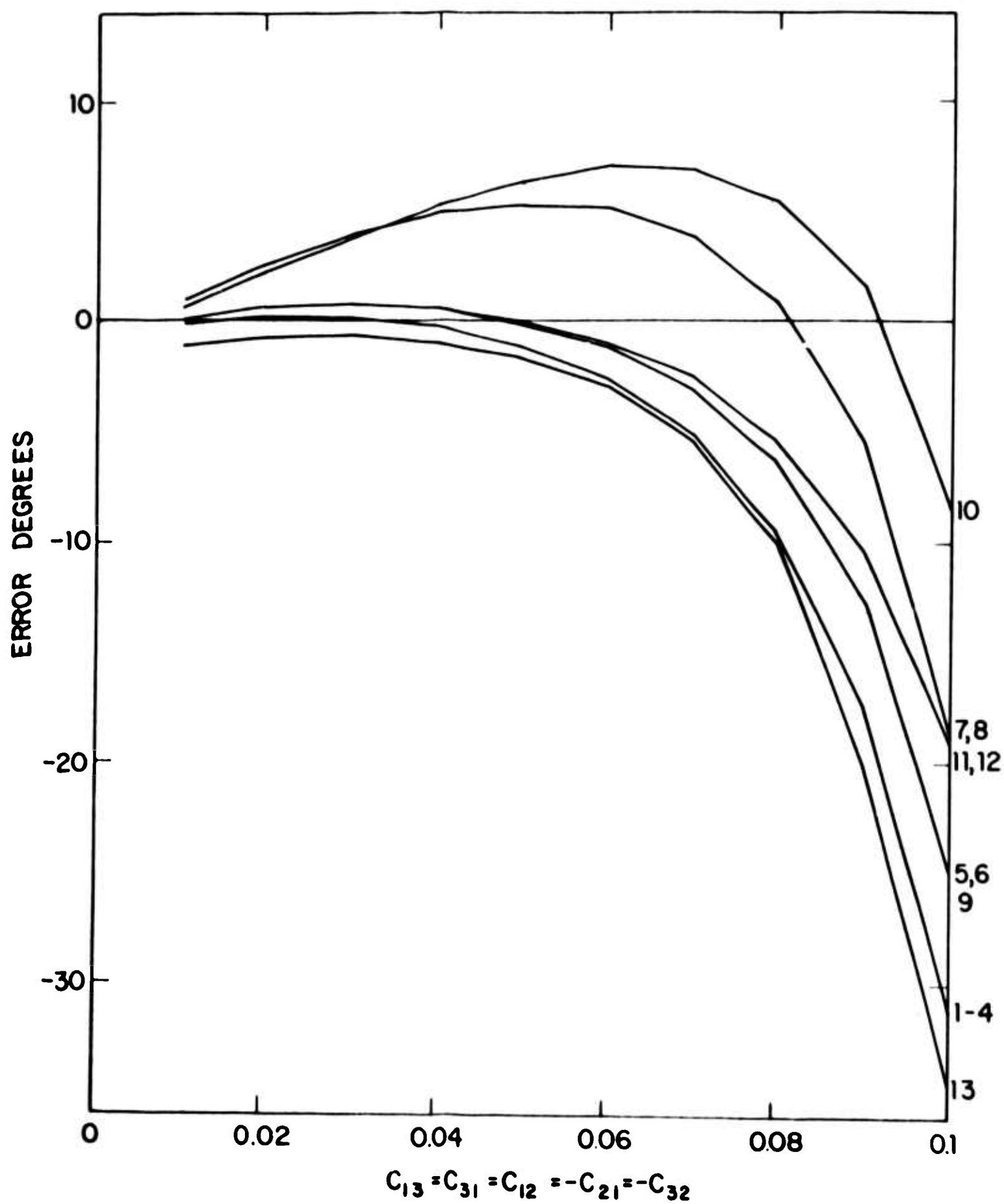
42

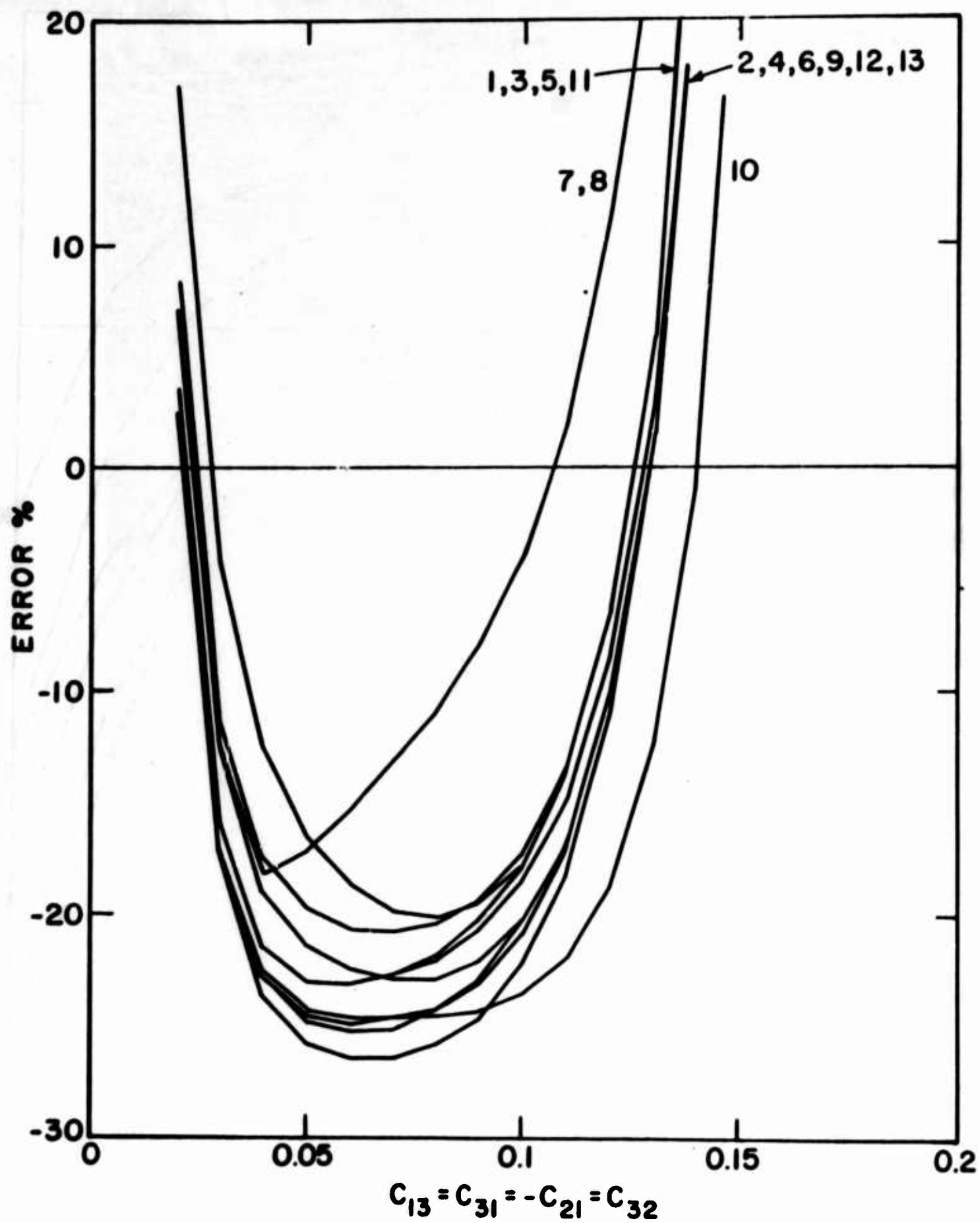Figure 14   Shear, Rotation and Compression, $\alpha = 2$ Angular Error

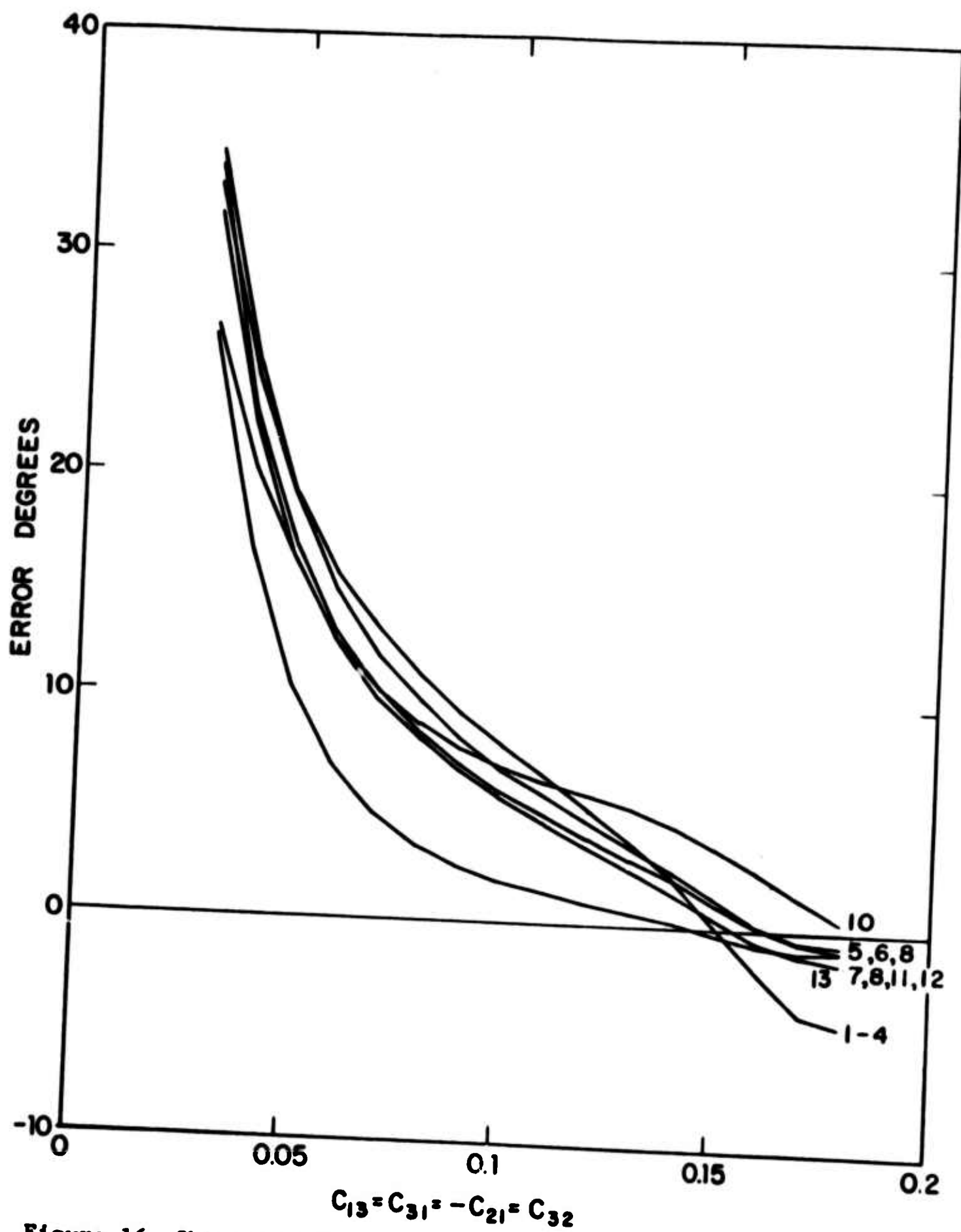Figure 15   Shear and Rotation, $\alpha = 2$ Magnitude Error

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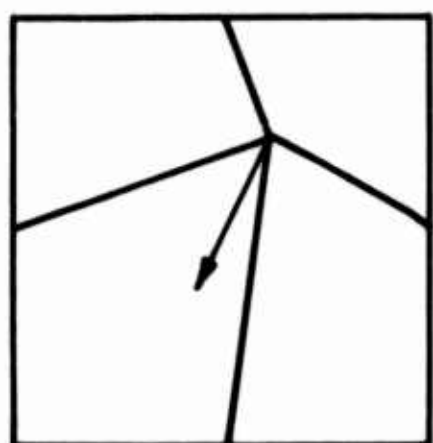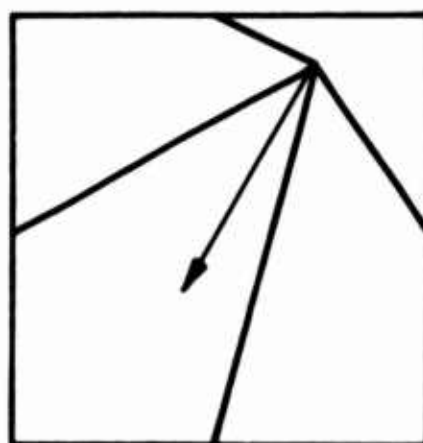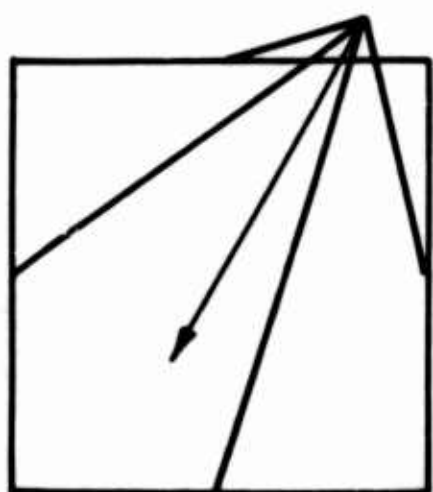Figure 16   Shear and Rotation, α = 2, Angular Error
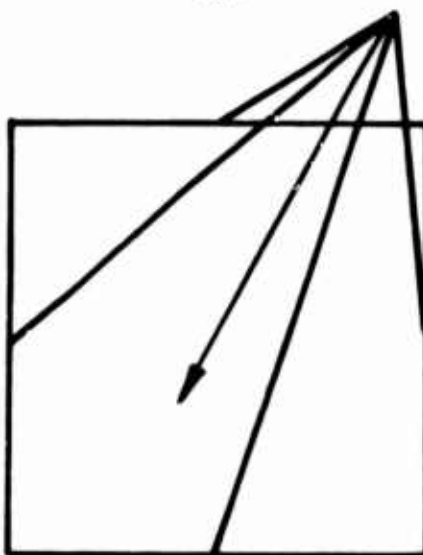
Figure 17 Configurations for Checking Sign Reversal

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